

STIC Search Report

Biotech-Chem Library

STIC Database Tracking Number: 146707

TO: Rei-Tsang Shiao
Location: 5a10 / 5c18
Monday, March 14, 2005
Art Unit: 1626
Phone: 571-272-0707
Serial Number: 10 / 622130

From: Jan Delaval
Location: Biotech-Chem Library
Remsen 1a51
Phone: 571-272-22504
jan.delaval@uspto.gov

Search Notes

Jan Belval
for search

Accession # 146707

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Robert (Raf) Shiao Examiner #: 79524 Date: 3/3/05
Art Unit: 1626 Phone Number: 2-0707 Serial Number: 10/622-130
Mail Box and Bldg/Room Location: 5A10/5C18 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc. if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of invention: Heterodiamondoids * any question please call me at 2-0707

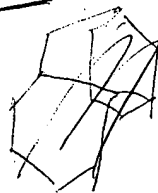
Inventors (please provide full names): Lia et al

Earliest Priority Filing Date: _____

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

I search a heterodiamondoid compound have a diamondoid nucleus selected from trimantane or tetramantane nucleus, and the nucleus has a atom selected from N, S, O (see Fig 1, 5, 6, 7, 8)

II search a compound (see Fig 2), of the ring structure and one of carbon atom is replaced by N, O, S, Se, B, P, As



STAFF USE ONLY

Searcher: Jan

Searcher Phone #: 22504

Searcher Location: 31405

Date Searcher Picked Up: 3/14/05

Date Completed: 3/14/05

Searcher Prep Review Time _____

Clerical Prep Time: 30

Online Time: + 90

Type of Search

NA Sequence (#) _____

AA Sequence (#) _____

Structure (#) ☒

Bibliographic _____

Litigation _____

Fulltext _____

Patent Family _____

Other _____

Vendors and cost where applicable

STN ☒

Dialog _____

Questel/Orbit ☒

Dr. Link _____

Lexis/Nexis _____

Sequence Systems _____

WWW/Internet _____

Other (specify) _____

=> d his

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FILE 'HCAPLUS' ENTERED AT 09:27:42 ON 10 MAR 2005

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E CHEVRON/PA,CS
L3 5478 S CHEVRON?/PA,CS
E CHEVRO/PA,CS
E LIU S/AU
L4 528 S E3,E12
E LIU SHENG/AU
L5 148 S E3,E16
E LIU SHENGGAO/AU
L6 22 S E3
E CARLSON R/AU
L7 88 S E3,E17,E18
E CARLSON ROB/AU
L8 163 S E4,E21-E25
E DAHL J/AU
L9 24 S E3,E7,E8
E DAHL JEREMY/AU
L10 32 S E3-E7
L11 77 S ?TETRAMANTAN? OR ?TRIAMANTAN?
L12 263 S ?DIAMONDOID?
L13 3 S L1,L3-L10 AND L2
L14 21 S L1,L3-L10 AND L11,L12
L15 21 S L13,L14
L16 5 S L15 AND ?ADAMANTAN?
L17 13 S L15 AND ?AMANTAN?
L18 13 S L16,L17
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L20 41 S L15-L19,L2
L21 37 S L12 AND L11
L22 98 S L12 AND ?AMANTAN?
L23 98 S L21,L22

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 L63 3 S L62 AND L1-L23
 L64 4 S L62,L63

FILE 'USPATFULL' ENTERED AT 10:23:27 ON 10 MAR 2005

L65 1 S L44

=> fil uspatful

FILE 'USPATFULL' ENTERED AT 10:23:48 ON 10 MAR 2005

CA INDEXING COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 8 Mar 2005 (20050308/PD)

FILE LAST UPDATED: 8 Mar 2005 (20050308/ED)

HIGHEST GRANTED PATENT NUMBER: US6865747

HIGHEST APPLICATION PUBLICATION NUMBER: US2005050605

CA INDEXING IS CURRENT THROUGH 8 Mar 2005 (20050308/UPCA)

ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 8 Mar 2005 (20050308/PD)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2005

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2005

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>>> USPAT2 is now available.  USPATFULL contains full text of the  <<<
>>> original, i.e., the earliest published granted patents or  <<<
>>> applications.  USPAT2 contains full text of the latest US  <<<
>>> publications, starting in 2001, for the inventions covered in  <<<
>>> USPATFULL.  A USPATFULL record contains not only the original  <<<
>>> published document but also a list of any subsequent  <<<
>>> publications.  The publication number, patent kind code, and  <<<
>>> publication date for all the US publications for an invention  <<<
>>> are displayed in the PI (Patent Information) field of USPATFULL  <<<
>>> records and may be searched in standard search fields, e.g., /PN, <<<
>>> /PK, etc.  <<<

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>>> classifications, or claims, that may potentially change from <<<
>>> the earliest to the latest publication. <<<
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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d l65 bib abs hitstr

L65 ANSWER 1 OF 1 USPATFULL on STN
AN 2004:77366 USPATFULL
TI Heterodiamondoids
IN Liu, Shenggao, Hercules, CA, UNITED STATES
Carlson, Robert M., Petaluma, CA, UNITED STATES
Dahl, Jeremy E., Palo Alto, CA, UNITED STATES
PA CHEVRON USA INC. (U.S. corporation)
PI US 2004059145 A1 20040325
AI US 2003-622130 A1 20030716 (10)
PRAI US 2002-397367P 20020718 (60)
DT Utility
FS APPLICATION
LREP William H. Benz, BURNS, DOANE, SWECKER & MATHIS, L.L.P., P.O. Box 1404,
Alexandria, VA, 22313-1404
CLMN Number of Claims: 37
ECL Exemplary Claim: 1
DRWN 51 Drawing Page(s)
LN.CNT 2469
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB This invention is related to heteroatom containing diamondoids (i.e., "heterodiamondoids") which are compounds having a diamondoid nucleus in which one or more of the diamondoid nucleus carbons has been substitutionally replaced with a noncarbon atom. These heteroatom substituents impart desirable properties to the diamondoid. In addition, the heterodiamondoids are functionalized affording compounds carrying one or more functional groups covalently pendant therefrom. This invention is further related to polymerizable functionalized heterodiamondoids. In a preferred aspect of this invention the diamondoid nuclei are triamantane and higher diamondoid nuclei. In another preferred aspect, the heteroatoms are selected to give rise to diamondoid materials which can serve as n- and p-type materials in electronic devices can serve as optically active materials.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

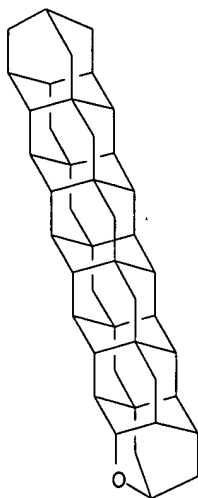
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652999-36-5 652999-38-7 652999-39-8
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, [1212121212] Azaundecamantane 652999-46-7, [1212121212]
Phosphaundecamantane 652999-47-8, [1212121212]
Arsaundecamantane

(calcn. of heat of formation; preparation of heterodiamondoids such as aza-,
oxa-, and thiatetramantane from fused adamantanes such as
tetramantanes)

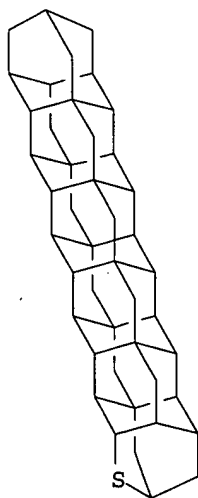
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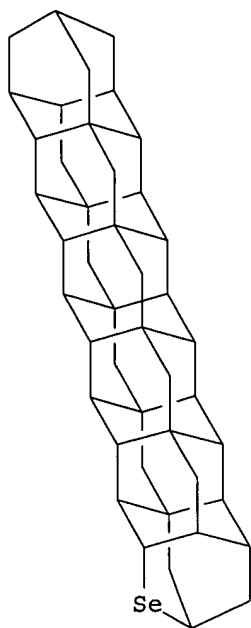
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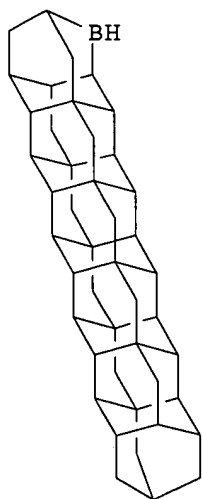


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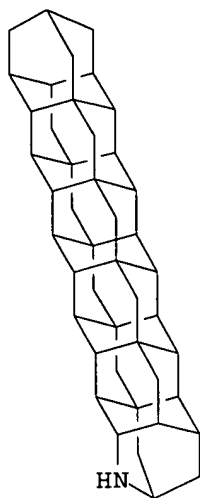
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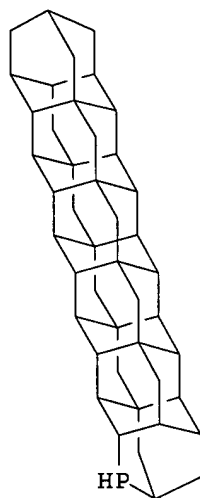
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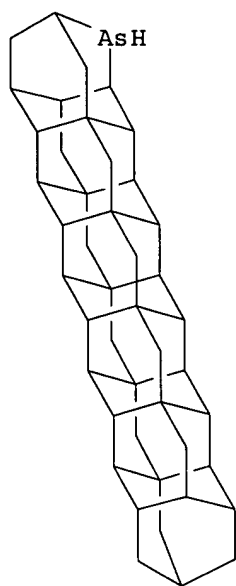
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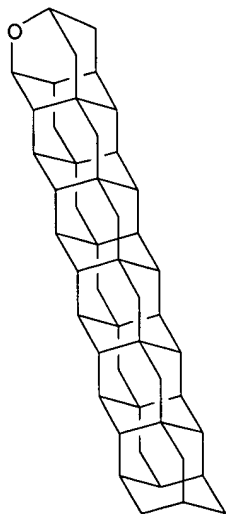
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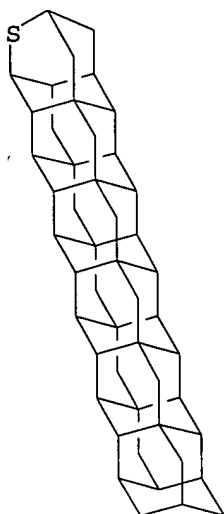
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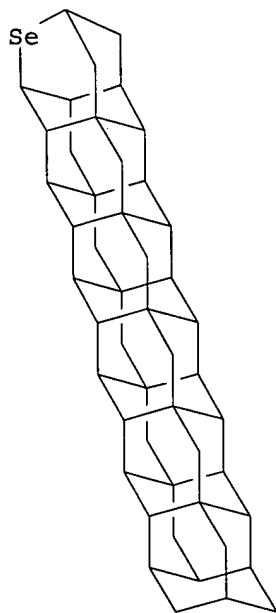
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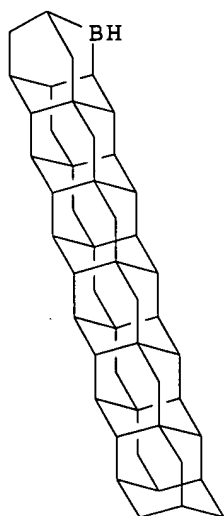
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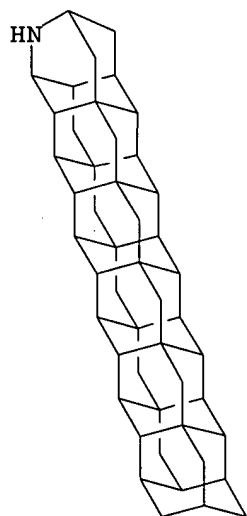
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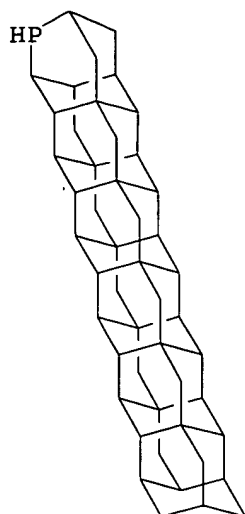
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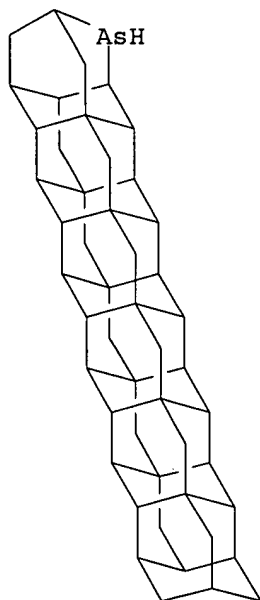
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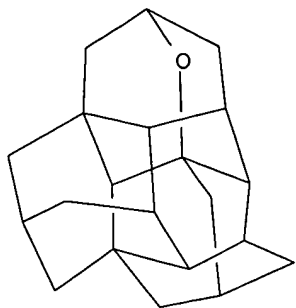
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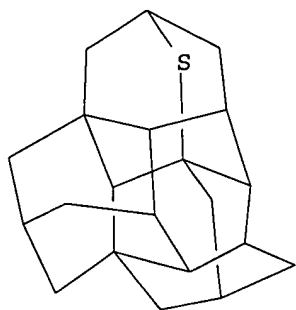


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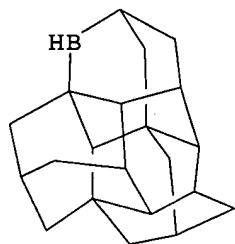
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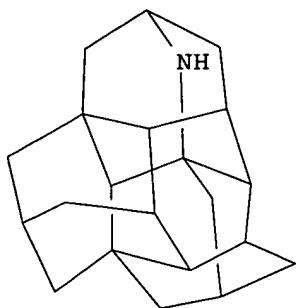
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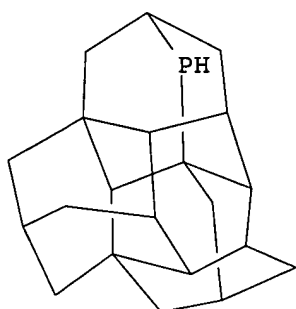
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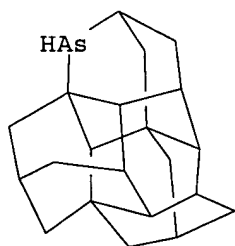
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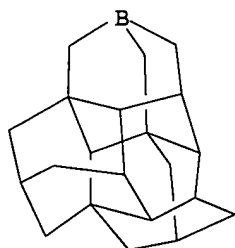
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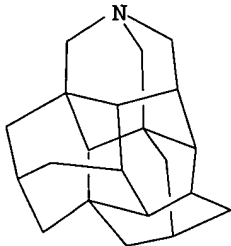
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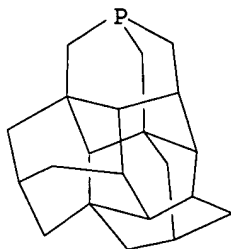
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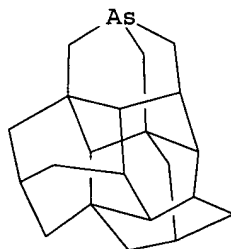
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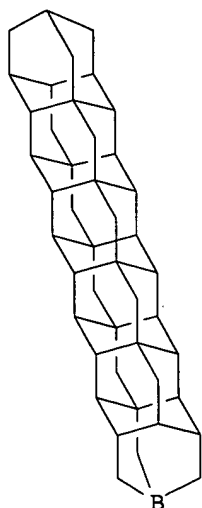
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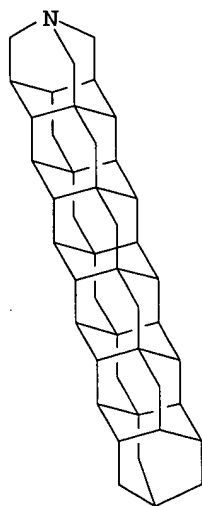


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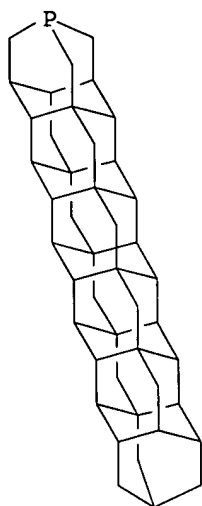
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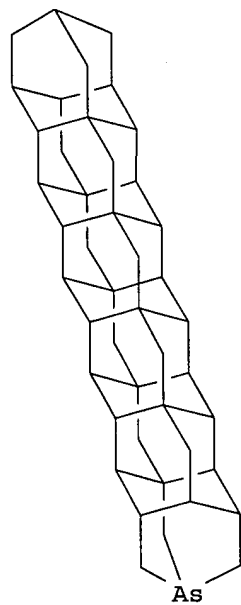
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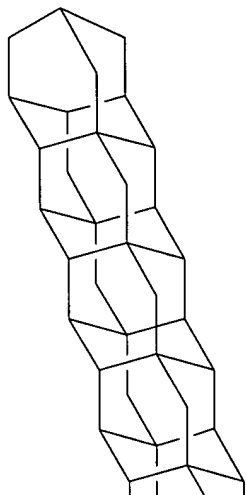


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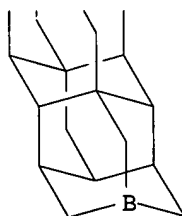


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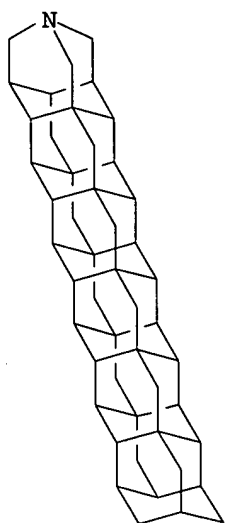
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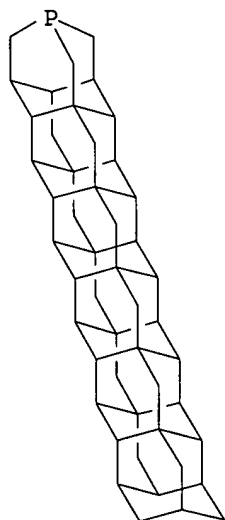
PAGE 2-A



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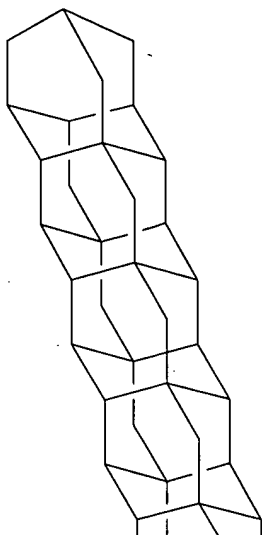


RN 652999-46-7 USPATFULL
CN [1212121212] Phosphaundecamantane (9CI) (CA INDEX NAME)

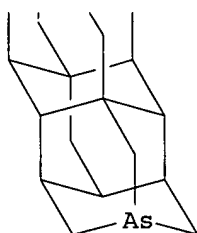


RN 652999-47-8 USPATFULL
CN [1212121212] Arsaundecamantane (9CI) (CA INDEX NAME)

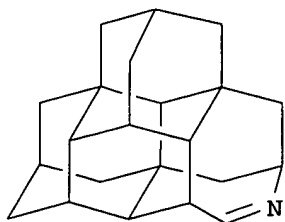
PAGE 1-A



PAGE 2-A

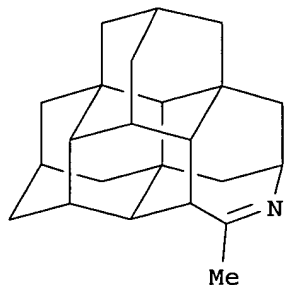


IT 652999-16-1P 652999-17-2P 652999-18-3P
 652999-19-4P 652999-20-7P 652999-23-0P
 652999-24-1P 652999-25-2P
 (preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane
 from fused adamantanes such as tetramantanes)
 RN 652999-16-1 USPATFULL
 CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylideneanthra[9,1-
 cd]azepine, 3,4,6,7,7a,8a,9,10,11,12a,12b,12c-dodecahydro- (9CI) (CA
 INDEX NAME)



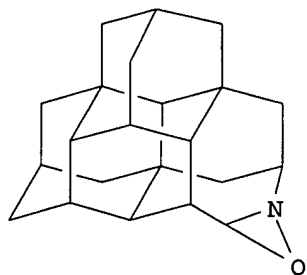
RN 652999-17-2 USPATFULL

CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylideneanthra[9,1-cd]azepine, 3,4,6,7,7a,8a,9,10,11,12a,12b,12c-dodecahydro-1-methyl- (9CI) (CA INDEX NAME)



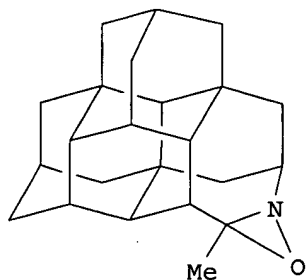
RN 652999-18-3 USPATFULL

CN 8H,9H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-5H-anthra[9,1-cd]oxazirino[2,3-a]azepine, dodecahydro- (9CI) (CA INDEX NAME)



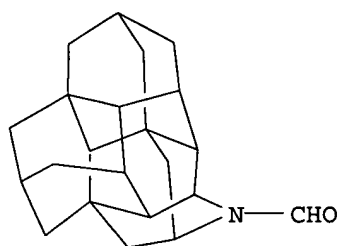
RN 652999-19-4 USPATFULL

CN 8H,9H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-5H-anthra[9,1-cd]oxazirino[2,3-a]azepine, dodecahydro-12c-methyl- (9CI) (CA INDEX NAME)



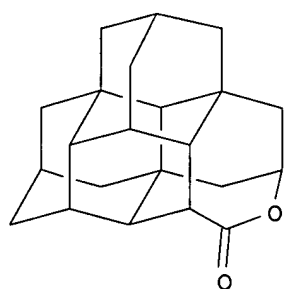
RN 652999-20-7 USPATFULL

CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-dibenzo[de,h]quinoline-1-carboxaldehyde, dodecahydro- (9CI) (CA INDEX NAME)



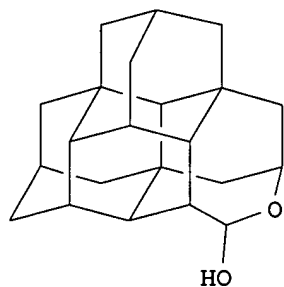
RN 652999-23-0 USPATFULL

CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-1H-anthra[9,1-cd]oxepin-1-one, dodecahydro- (9CI) (CA INDEX NAME)



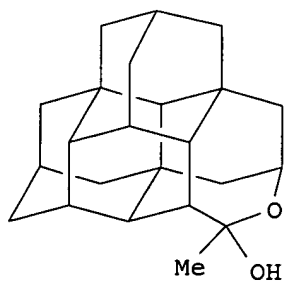
RN 652999-24-1 USPATFULL

CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-1H-anthra[9,1-cd]oxepin-1-ol, dodecahydro- (9CI) (CA INDEX NAME)



RN 652999-25-2 USPATFULL

CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-1H-anthra[9,1-cd]oxepin-1-ol, dodecahydro-1-methyl- (9CI) (CA INDEX NAME)

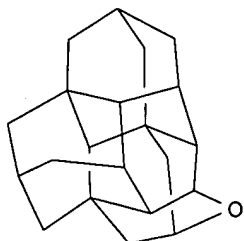


IT 652999-15-0P 652999-21-8P 652999-32-1P

(preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane from fused adamantanes such as tetramantanes)

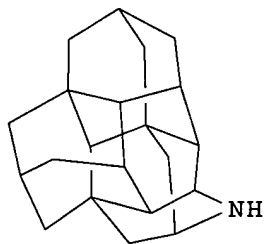
RN 652999-15-0 USPATFULL

CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[9,1-bc]pyran, dodecahydro- (9CI) (CA INDEX NAME)



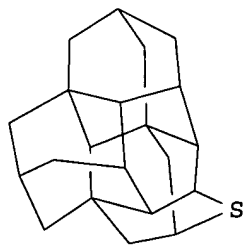
RN 652999-21-8 USPATFULL

CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-dibenzo[de,h]quinoline, dodecahydro- (9CI) (CA INDEX NAME)



RN 652999-32-1 USPATFULL

CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[9,1-bc]thiopyran, dodecahydro- (9CI) (CA INDEX NAME)



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FILE LAST UPDATED: 9 Mar 2005 (20050309/ED)

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L64 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:641668 HCAPLUS
DN 141:320341
ED Entered STN: 10 Aug 2004
TI Diamond fragments as building blocks of functional nanostructures
AU McIntosh, Gregory C.; Yoon, Mina; Berber, Savas; Tomanek, David
CS Naval Base, Defence Technology Agency, Auckland, N. Z.
SO Physical Review B: Condensed Matter and Materials Physics (2004), 70(4),
045401/1-045401/8
CODEN: PRBMDO; ISSN: 0163-1829
PB American Physical Society
DT Journal
LA English
CC 65-3 (General Physical Chemistry)
AB Using d. functional theory, we investigate the equilibrium structure,
stability, and electronic properties of nanostructured,
hydrogen-terminated diamond fragments. The equilibrium atomic arrangement and
electronic structure of these nanostructures turn out to be very similar
to bulk diamond. We find that such **diamondoids** may enter
spontaneously into carbon nanotubes. Polymerization inside a nanotube is
favored
especially when boron and nitrogen are substituted for carbon atoms.
ST **diamondoid** nanostructure electronic structure stability
IT LUMO (molecular orbital)
(HOMO gap; diamond fragments as building blocks of functional
nanostructures studied by DFT)
IT HOMO (molecular orbital)
(LUMO gap; diamond fragments as building blocks of functional
nanostructures studied by DFT)
IT Bond length
(carbon-carbon; diamond fragments as building blocks of functional
nanostructures studied by DFT)
IT Nanotubes
(carbon; diamond fragments as building blocks of functional
nanostructures studied by DFT)
IT Band gap
Band structure
Binding energy
Cluster model
Conduction band
Density of states
Electron density
HOMO (molecular orbital)
LUMO (molecular orbital)
Nanostructures
Polymerization
Valence band

(diamond fragments as building blocks of functional nanostructures studied by DFT)

IT Energy

(formation; diamond fragments as building blocks of functional nanostructures studied by DFT)

IT 281-23-2, **Adamantane** 2292-79-7, **Diamantane**
7782-40-3, **Diamond**, properties 27745-90-0, **Tetramantane**
112761-65-6, **Decamantane** **765943-15-5**
765943-16-6

RL: PRP (Properties)

(diamond fragments as building blocks of functional nanostructures studied by DFT)

RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD

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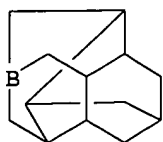
IT **765943-15-5** **765943-16-6**

RL: PRP (Properties)

(diamond fragments as building blocks of functional nanostructures studied by DFT)

RN 765943-15-5 HCAPLUS

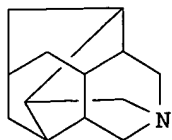
CN 1H-2,8,4,6-[1,2,3,4]Butanetetrayl-2-benzoborin, octahydro- (9CI) (CA INDEX NAME)



RN 765943-16-6 HCAPLUS

CN 1H-2,8,4,6-[1,2,3,4]Butanetetraylisoquinoline, octahydro- (9CI) (CA INDEX

NAME)



L64 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2004:365485 HCAPLUS
 DN 141:318401
 ED Entered STN: 05 May 2004
 TI Theoretical analysis of diamond mechanosynthesis. Part II. C2 mediated growth of diamond C(110) surface via Si/Ge-triadamantane dimer placement tools
 AU Mann, David J.; Peng, Jingping; Freitas, Robert A., Jr.; Merkle, Ralph C.
 CS Zyvex Corp., Richardson, TX, 75081, USA
 SO Journal of Computational and Theoretical Nanoscience (2004), 1(1), 71-80
 CODEN: JCTNAB; ISSN: 1546-1955
 PB American Scientific Publishers
 DT Journal
 LA English
 CC 57-8 (Ceramics)
 Section cross-reference(s): 66, 75
 AB This paper presents a computational and theor. investigation of the vacuum mechanosynthesis of diamond on the clean C(110) surface from carbon dimer (C2) precursors positionally constrained throughout the reaction pathway by silicon- or germanium-doped triadamantane derivs. mounted on a scanning probe tip. Interactions between the dimer placement tools and the bare diamond C(110) surface are investigated using D. Functional Theory (DFT) with generalized gradient approximation (GGA) by constructing the reaction path potential energy profiles and analyzing ab initio mol. dynamics simulations. Similar methods are applied to study the energetics and kinetics of recharging the tool with acetylene. Mol. mechanics simulations on extended tool tips are carried out to elucidate the positional uncertainty of the carbon dimer due to thermal fluctuations, and the possibility of intermol. dimerization and dehydrogenation of the dimer placement tools is explored.
 ST diamond growth dicarbon precursor
 IT Simulation and Modeling, physicochemical
 (mol. dynamics; theor. study of C2 mediated growth of diamond C(110) surface for anal. of diamond mechanosynthesis via Si/Ge-triadamantane dimer placement tools)
 IT Reaction mechanism
 (surface; theor. study of C2 mediated growth of diamond C(110) surface for anal. of diamond mechanosynthesis via Si/Ge-triadamantane dimer placement tools)
 IT Mechanochemical reaction
 Surface structure
 (theor. study of C2 mediated growth of diamond C(110) surface for anal. of diamond mechanosynthesis via Si/Ge-triadamantane dimer placement tools)
 IT 7782-40-3, Diamond, processes
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
 (theor. study of C2 mediated growth of diamond C(110) surface for anal. of diamond mechanosynthesis via Si/Ge-triadamantane dimer placement tools)
 IT 681029-68-5 681029-69-6
 RL: PRP (Properties)

(theor. study of C2 mediated growth of diamond C(110) surface for anal.
of diamond mechanosynthesis via Si/Ge-triadamantane dimer placement
tools)

IT 12070-15-4, Carbon dimer

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)

(theor. study of C2 mediated growth of diamond C(110) surface for anal.
of diamond mechanosynthesis via Si/Ge-triadamantane dimer placement
tools)

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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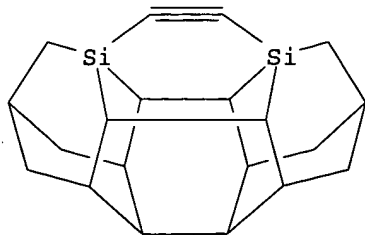
IT 681029-68-5 681029-69-6

RL: PRP (Properties)

(theor. study of C2 mediated growth of diamond C(110) surface for anal.
of diamond mechanosynthesis via Si/Ge-triadamantane dimer placement
tools)

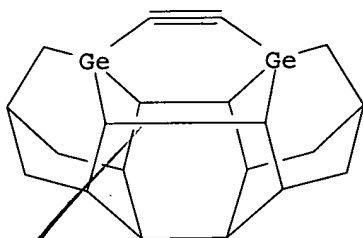
RN 681029-68-5 HCAPLUS

CN Disila[6]fulleroid-C22, tetrahydro- (9CI) (CA INDEX NAME)



RN 681029-69-6 HCAPLUS

CN Digerma[6]fulleroid-C22, tetrahydro- (9CI) (CA INDEX NAME)



L64 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2004:80675 HCAPLUS
 DN 140:146009
 ED Entered STN: 01 Feb 2004
 TI Preparation of **heterodiamondoids** from fused **adamantanes**
 IN **Liu, Shenggao; Carlson, Robert M.**
 PA **Chevron U.S.A. Inc., USA; Dahl, Jeremy E.**
 SO PCT Int. Appl., 134 pp.
 CODEN: PIXXD2

DT Patent
 LA English
 IC ICM C07D311-78
 ICS C07D313-06; C07D335-04; C07D221-18
 CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
 Section cross-reference(s): 76

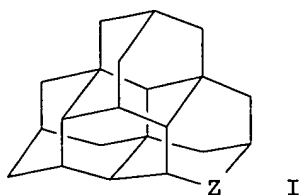
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004009577	A1	20040129	WO 2003-US22483	20030717 <--
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	US 2004059145	A1	20040325	US 2003-622130	20030716 <--
PRAI	US 2002-397367P	P	20020718	<--	
	US 2002-397368P	P	20020718		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2004009577	ICM	C07D311-78
	ICS	C07D313-06; C07D335-04; C07D221-18
US 2004059145	ECLA	C07C023/20; C07C049/423; C07C049/617; C07C061/29; C07D221/22; C07D311/96; C07D313/06; C07D335/04; C07D471/10+221C+221C+9; C07F009/6568C

OS MARPAT 140:146009
 GI



- AB This invention is related to heteroatom containing **diamondoids** (i.e., '**heterodiamondoids**'), e.g. **azatetramantane**, **oxatetramantane**, and **thiatetramantane** (I; X = NH, O, S), which are compds. having a **diamondoid** nucleus in which one or more of the **diamondoid** nucleus carbons has been substitutionally replaced with a noncarbon atom. These heteroatom substituents impart desirable properties to the **diamondoid**. In addition, the **heterodiamondoids** are functionalized affording compds. carrying one or more functional groups covalently pendant therefrom. This invention is further related to polymerizable functionalized **heterodiamondoids**. In a preferred aspect of this invention the **diamondoid** nuclei are **triamantane** and higher **diamondoid** nuclei. In another preferred aspect, the heteroatoms are selected to give rise to **diamondoid** materials which can serve as n- and p-type materials in electronic devices and in optical devices as optically active materials (no data).
- ST **heterodiamondoid** prepn; **azatetramantane**
oxatetramantane **thiatetramantane** prepn
- IT Formation enthalpy
(preparation of **heterodiamondoids** such as aza-, oxa-, and **thiatetramantane** from fused **adamantanes** such as **tetramantanes**)
- IT Heterocyclic compounds
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of **heterodiamondoids** such as aza-, oxa-, and **thiatetramantane** from fused **adamantanes** such as **tetramantanes**)
- IT 652998-89-5, [121212121] **Decamantane** 652998-90-8, [121212121] **Oxadecamantane** 652998-91-9, [121212121] **Thiadecamantane** 652998-92-0, [121212121] **Selenadecamantane** 652998-93-1, [121212121] **Boradecamantane** 652998-94-2, [121212121] **Azadecamantane** 652998-95-3, [121212121] **Phosphadecamantane** 652998-96-4, [121212121] **Arsadecamantane** 652998-97-5, [121212121] **Undecamantane** 652998-98-6, [121212121] **Oxaundecamantane** 652998-99-7, [121212121] **Thiaundecamantane** 652999-00-3, [121212121] **Selenaundecamantane** 652999-01-4, [121212121] **Boraundecamantane** 652999-02-5, [121212121] **Azaundecamantane** 652999-03-6, [121212121] **Phosphaundecamantane** 652999-04-7, [121212121] **Arsaundecamantane** 652999-05-8 652999-06-9 652999-07-0 652999-08-1 652999-09-2 652999-11-6 652999-12-7 652999-35-4 652999-36-5 652999-38-7 652999-39-8 652999-40-1, [121212121] **Boradecamantane** 652999-41-2, [121212121] **Azadecamantane** 652999-42-3, [121212121] **Phosphadecamantane** 652999-43-4, [121212121] **Arsadecamantane** 652999-44-5, [121212121] **Boraundecamantane** 652999-45-6, [121212121] **Azaundecamantane** 652999-46-7, [121212121]

Phosphaundecamantane 652999-47-8, [1212121212]

Arsaundecamantane

RL: PRP (Properties)

(calcn. of heat of formation; preparation of **heterodiamondoids** such as aza-, oxa-, and **thiatetramantane** from fused **adamantanes** such as **tetramantanes**)

IT 917-54-4, Methyllithium 27745-90-0 73635-95-7 73635-96-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of **heterodiamondoids** such as aza-, oxa-, and **thiatetramantane** from fused **adamantanes** such as **tetramantanes**)

IT 546101-72-8P 546102-13-0P 652999-13-8P 652999-14-9P

652999-16-1P 652999-17-2P 652999-18-3P

652999-19-4P 652999-20-7P 652999-23-0P

652999-24-1P 652999-25-2P 652999-26-3P 652999-27-4P

652999-29-6P 652999-30-9P 652999-31-0P 652999-33-2P 652999-34-3P

653570-14-0P 653570-15-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of **heterodiamondoids** such as aza-, oxa-, and **thiatetramantane** from fused **adamantanes** such as **tetramantanes**)

IT 652999-15-0P 652999-21-8P 652999-22-9P 652999-28-5P

652999-32-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of **heterodiamondoids** such as aza-, oxa-, and **thiatetramantane** from fused **adamantanes** such as **tetramantanes**)

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Chapman, O; US 5019660 A 1991 HCAPLUS

(2) Dahl, J; WO 02057201 A 2002 HCAPLUS

(3) Dahl, J; WO 02058139 A 2002 HCAPLUS

(4) Dahl, J; WO 03050066 A 2003 HCAPLUS

(5) Fritz, G; ANGEWANDTE CHEMIE, INTERNATIONAL EDITION IN ENGLISH 1970, V9(6), P464 HCAPLUS

(6) Fritz, G; ZEITSCHRIFT FUER ANORGANISCHE UND ALLGEMEINE CHEMIE 1984, V512, P103 HCAPLUS

(7) Marchand, A; SCIENCE 2003, V299(5603), P52 HCAPLUS

(8) Mobil Oil Corp; WO 9506019 A 1995 HCAPLUS

(9) Mochizuki, Y; CHEMICAL PHYSICS LETTERS 2001, V336(5,6), P451 HCAPLUS

IT 652998-90-8, [121212121] **Oxadecamantane**

652998-91-9, [121212121] **Thiadecamantane**

652998-92-0, [121212121] **Selenadecamantane**

652998-93-1, [121212121] **Boradecamantane**

652998-94-2, [121212121] **Azadecamantane**

652998-95-3, [121212121] **Phosphadecamantane**

652998-96-4, [121212121] **Arsadecamantane**

652998-98-6, [121212121] **Oxaundecamantane**

652998-99-7, [121212121] **Thiaundecamantane**

652999-00-3, [121212121] **Selenaundecamantane**

652999-01-4, [121212121] **Boraundecamantane**

652999-02-5, [121212121] **Azaundecamantane**

652999-03-6, [121212121] **Phosphaundecamantane**

652999-04-7, [121212121] **Arsaundecamantane**

652999-05-8 652999-06-9 652999-08-1

652999-09-2 652999-11-6 652999-12-7

652999-35-4 652999-36-5 652999-38-7

652999-39-8 652999-40-1, [121212121]

Boradecamantane 652999-41-2, [121212121]

Azadecamantane 652999-42-3, [121212121]

Phosphadecamantane 652999-43-4, [121212121]

Arsadecamantane 652999-44-5, [121212121]

Boraundecamantane 652999-45-6, [1212121212]

Azaundecamantane 652999-46-7, [1212121212]

Phosphaundecamantane 652999-47-8, [1212121212]

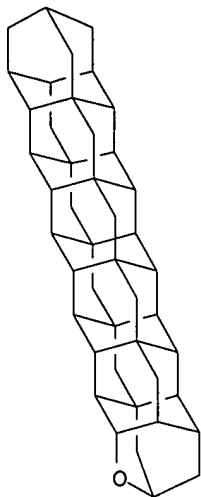
Arsaundecamantane

RL: PRP (Properties)

(calcn. of heat of formation; preparation of **heterodiamondoids**
such as aza-, oxa-, and **thiatetramantane** from fused
adamantanes such as **tetramantanes**)

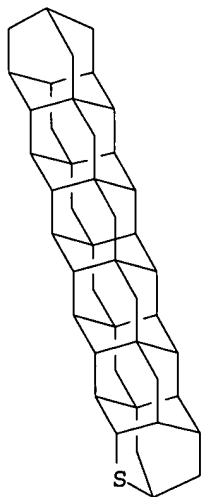
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CN [121212121] Oxadecamantane (9CI) (CA INDEX NAME)



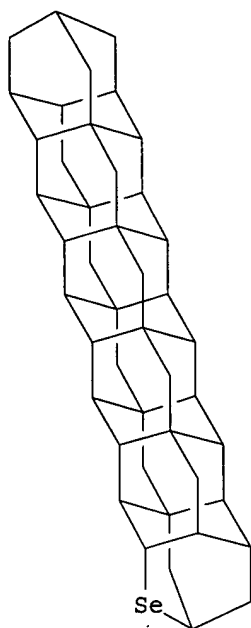
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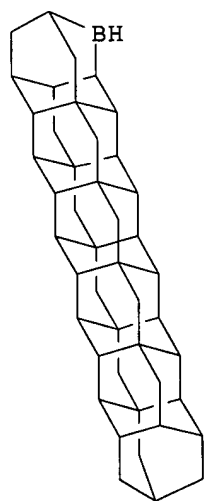


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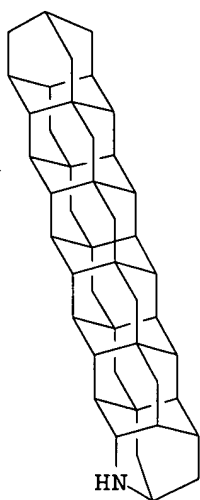
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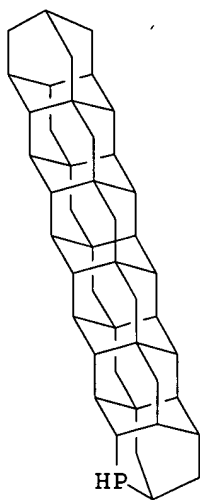
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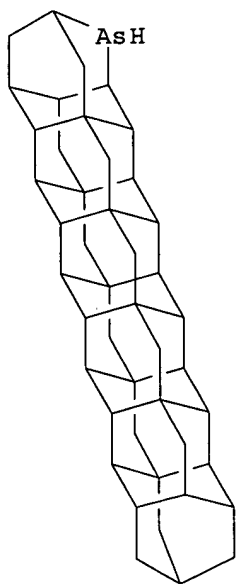
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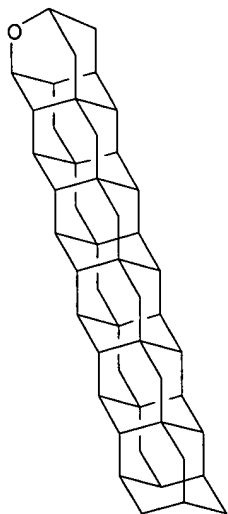
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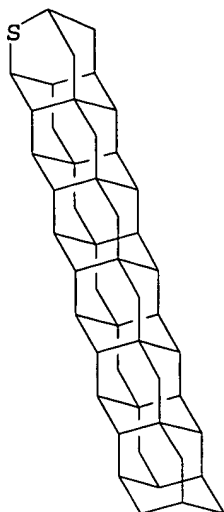
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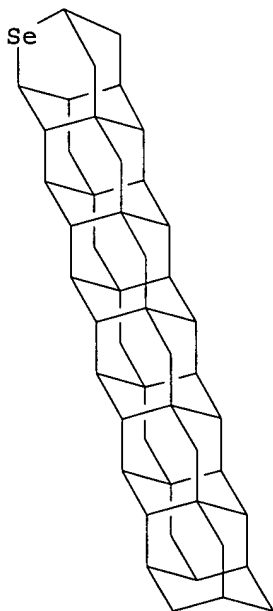
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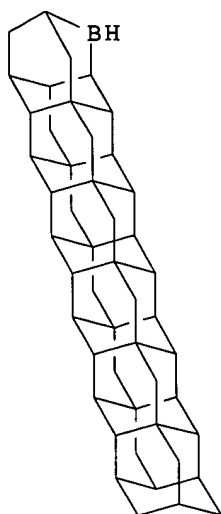
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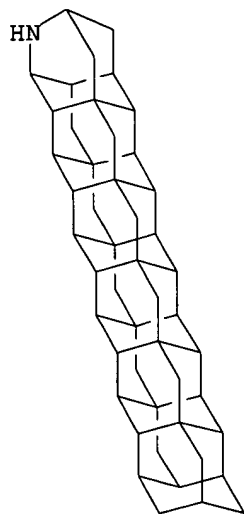
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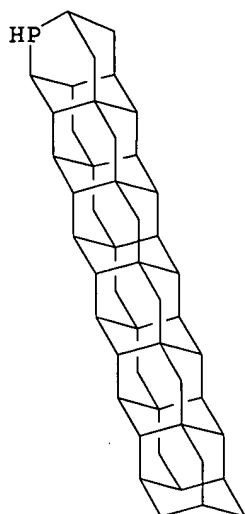
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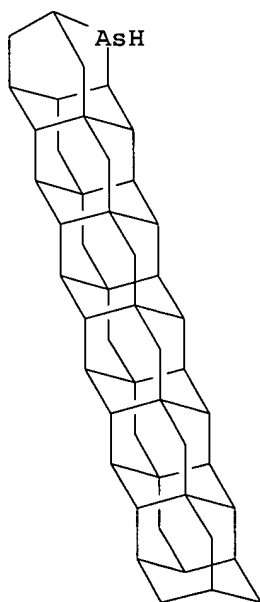
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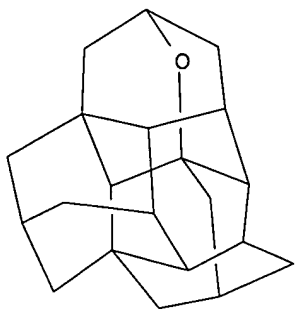
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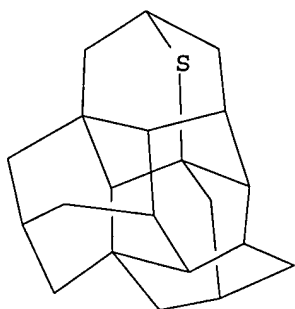
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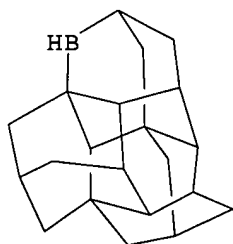
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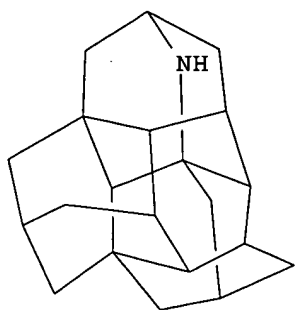
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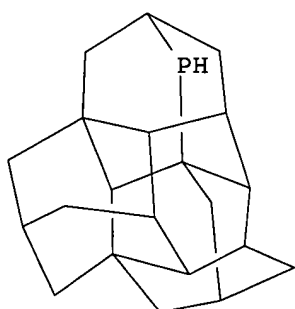
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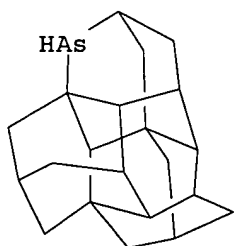
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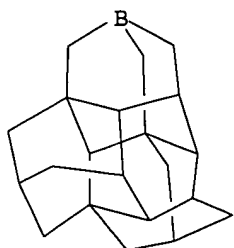
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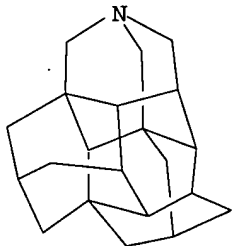
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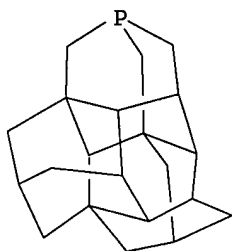
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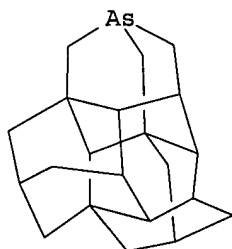
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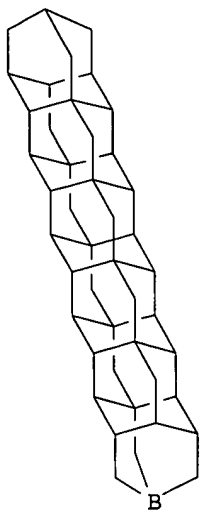
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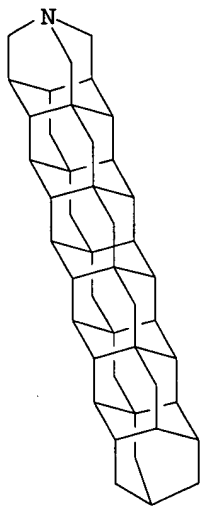
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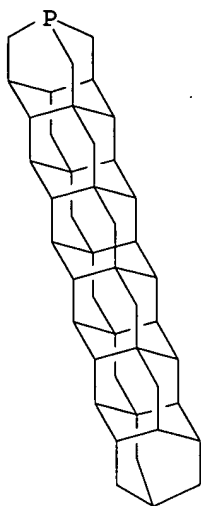
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CN [121212121] Boradecamantane (9CI) (CA INDEX NAME)



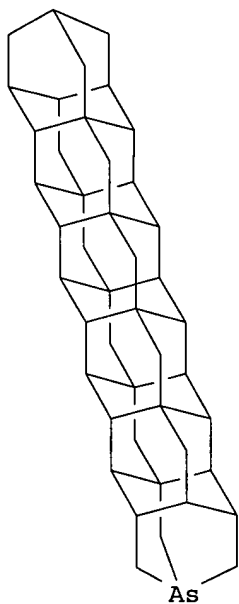
RN 652999-41-2 HCAPLUS
CN [121212121] Azadecamantane (9CI) (CA INDEX NAME)



RN 652999-42-3 HCAPLUS
CN [121212121] Phosphadecamantane (9CI) (CA INDEX NAME)

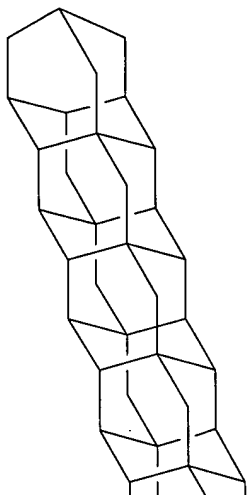


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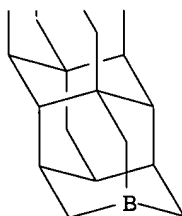


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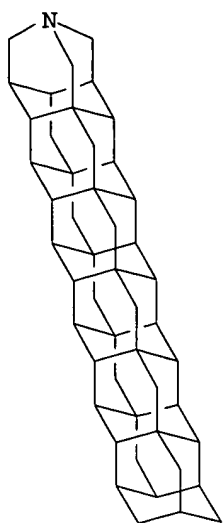
PAGE 1-A



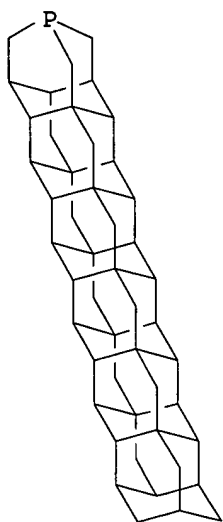
PAGE 2-A



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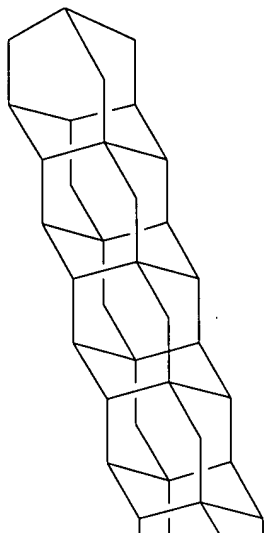


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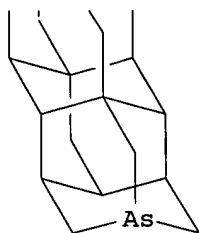


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CN [1212121212] Arsaundecamantane (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



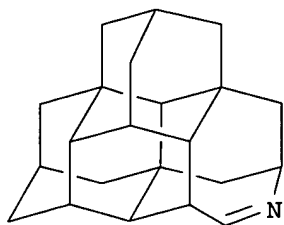
IT 652999-16-1P 652999-17-2P 652999-18-3P
 652999-19-4P 652999-20-7P 652999-23-0P
 652999-24-1P 652999-25-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

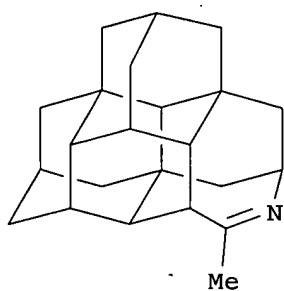
(preparation of **heterodiamondoids** such as aza-, oxa-, and
thiatetramantane from fused **adamantanes** such as
tetramantanes)

RN 652999-16-1 HCAPLUS

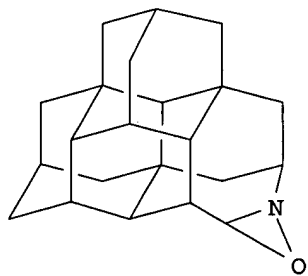
CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylideneanthra[9,1-
 cd]azepine, 3,4,6,7,7a,8a,9,10,11,12a,12b,12c-dodecahydro- (9CI) (CA
 INDEX NAME)



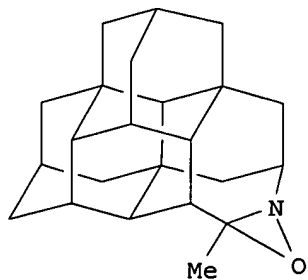
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 (CA INDEX NAME)



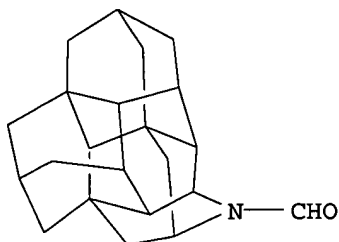
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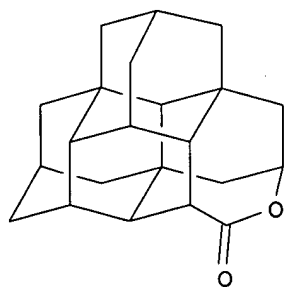
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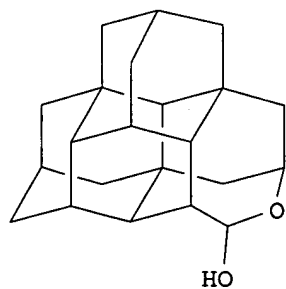
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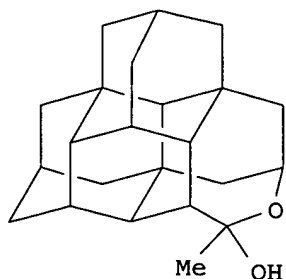
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RN 652999-24-1 HCAPLUS
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RN 652999-25-2 HCAPLUS
 CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylidene-1H-anthra[9,1-cd]oxepin-1-ol, dodecahydro-1-methyl- (9CI) (CA INDEX NAME)

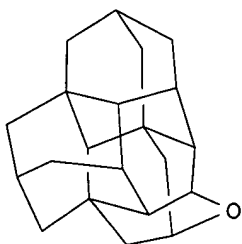


IT 652999-15-0P 652999-21-8P 652999-32-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of **heterodiamondoids** such as aza-, oxa-, and
thiatetramantane from fused **adamantanes** such as
tetramantanes)

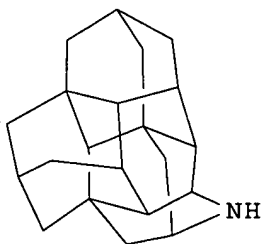
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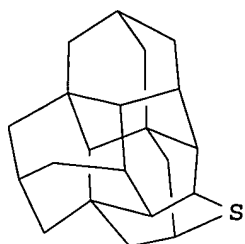
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RN 652999-32-1 HCAPLUS

CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[9,1-bc]thiopyran, dodecahydro- (9CI) (CA INDEX NAME)



L64 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2003:800853 HCAPLUS
 DN 140:339373
 ED Entered STN: 13 Oct 2003
 TI Theoretical analysis of a carbon-carbon dimer placement tool for diamond
 mechanosynthesis
 AU Merkle, Ralph C.; Freitas, Robert A., Jr.
 CS Zyvex Corp., Richardson, TX, USA
 SO Journal of Nanoscience and Nanotechnology (2003), 3(4), 319-324
 CODEN: JNNOAR; ISSN: 1533-4880
 PB American Scientific Publishers
 DT Journal
 LA English
 CC 29-6 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 22, 24
 AB D. functional theory is used with Gaussian 98 to analyze a new family of
 proposed mechanosynthetic tools that could be employed for the placement
 of two carbon atoms-a carbon-carbon (CC) dimer-on a growing diamond
 surface at a specific site. Optimized structures and potential energies
 were calculated for 5,5'-ethynediyl-bridged 2,2',4,4',9,9'-
biadamantane and its 5,5'-disila-, 5,5'-digerma-, 5,5'-distanna-,
 5,5'-diplumba- and 5-sila-5-germa-analogs. The stationary points for the
 5,5'-ethynediyl-, 5,5'-ethyldiyne carbene and 2,2',4,4',5,5',9,9'-
biadamantanes were located. The anal. focuses on specific Group
 IV-substituted **biadamantane** tool tip structures and evaluates
 their stability and the strength of the bond they make with the CC dimer.
 These tools should be stable in a vacuum and should be able to hold and
 position a CC dimer in a manner suitable for positionally controlled
 diamond mechanosynthesis at room temperature
 ST **biadamantane** sila germa stanna plumba ethynediyl DFT geometry
 energy; carbon dimer placement tool **biadamantane** alkyne geometry
 potential energy; polycyclic compd condensed **adamantane**
biadamantane heterocycle ethynediyl DFT calcn; heterocyclic compd
 silicon germanium tin lead polycyclic DFT energy; DFT geometry energy
 polycyclic **adamantane** Group IVA deriv calcn; diamond
diamondoid hydrocarbon **diadamantane** hetero substituted
 DFT geometry energy; mol structure optimized hetero **diadamantane**
 ethynediyl linked
 IT Density functional theory
 (B3LYP; geometry optimization and potential energy of ethynediyl-linked
heterobiadamantanes as carbon dimer precursors)
 IT Potential energy
 (DFT B3LYP geometry optimization and potential energy of
 ethynediyl-linked **heterobiadamantanes** as carbon dimer
 precursors)
 IT Carbenes (methylene derivatives)
 RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation,
 nonpreparative)
 (DFT B3LYP geometry optimization and potential energy of
 ethynediyl-linked **heterobiadamantanes** as carbon dimer

- precursors)
- IT Bond energy
(carbon-heteroatom bond energy of ethynediyl-linked **heterobiadamantanes** as carbon dimer precursors)
- IT Dimers
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(carbon; DFT geometry optimization and potential energy of ethynediyl-linked **heterobiadamantanes** as carbon dimer precursors)
- IT Hydrocarbons, properties
RL: PRP (Properties)
(**diamondoid**, **biadamantanes**; DFT B3LYP geometry optimization and potential energy of ethynediyl-linked **heterobiadamantanes** as carbon dimer precursors)
- IT Group IVA element compounds
RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(**heterobiadamantanes**; DFT B3LYP geometry optimization and potential energy of ethynediyl-linked **heterobiadamantanes** as carbon dimer precursors)
- IT Molecular structure
(optimized; of ethynediyl-linked **heterobiadamantanes** as carbon dimer precursors)
- IT Polycyclic compounds
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(tricyclic; DFT B3LYP geometry optimization and potential energy of ethynediyl-linked **heterobiadamantanes** as carbon dimer precursors)
- IT 681029-73-2P 681029-74-3P 681029-75-4P
681029-76-5P 681029-77-6P
RL: BYP (Byproduct); PRP (Properties); PREP (Preparation)
(DFT B3LYP geometry optimization and potential energy of ethynediyl-linked **heterobiadamantanes** as carbon dimer precursors)
- IT 681029-78-7, [4,6]Fulleroid-C20 681029-79-8,
Disila[4,6]fulleroid-C20 681029-80-1, Digerma[4,6]fulleroid-C20
681029-81-2, Distanna[4,6]fulleroid-C20 681029-82-3,
Diplumba[4,6]fulleroid-C20 681029-83-4, Germasila[4,6]fulleroid-C20
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(DFT B3LYP geometry optimization and potential energy of ethynediyl-linked **heterobiadamantanes** as carbon dimer precursors)
- IT 681029-67-4 681029-68-5 681029-69-6
681029-70-9 681029-71-0 681029-72-1
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(fragmentation; DFT B3LYP geometry optimization and potential energy of ethynediyl-linked **heterobiadamantanes** as carbon dimer precursors)

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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- (17) Page, M; J Am Chem Soc 1991, V113, P3270 HCAPLUS
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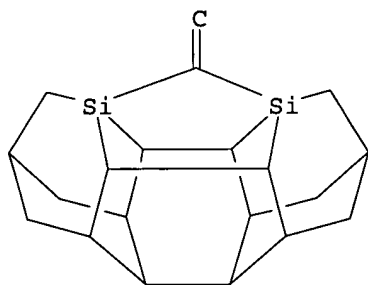
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RL: BYP (Byproduct); PRP (Properties); PREP (Preparation)
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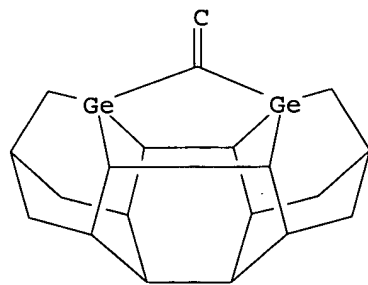
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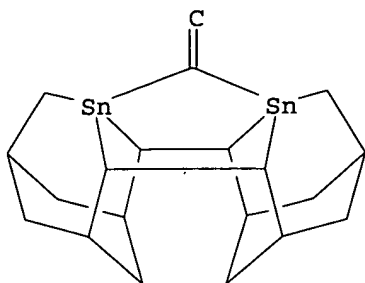
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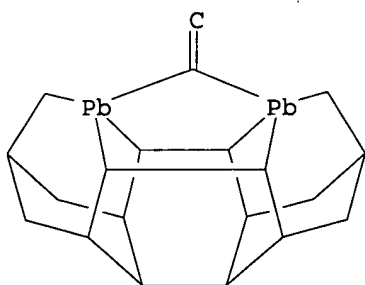


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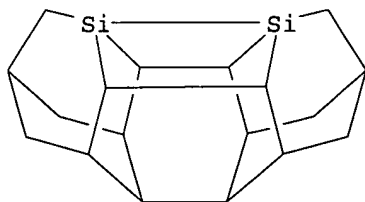
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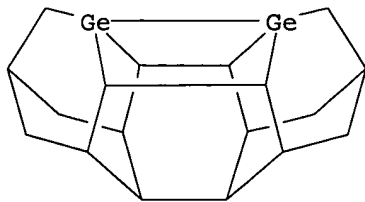
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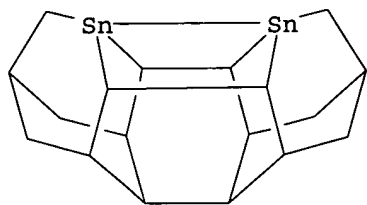
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 RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation,
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 (DFT B3LYP geometry optimization and potential energy of
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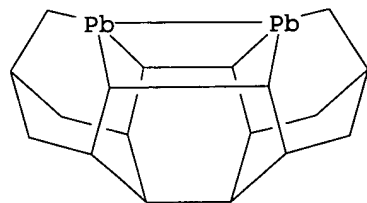
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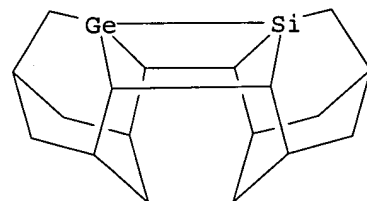
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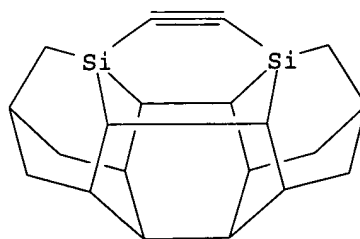
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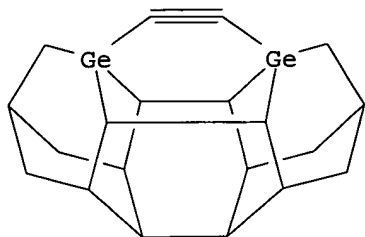
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RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
 (fragmentation; DFT B3LYP geometry optimization and potential energy of
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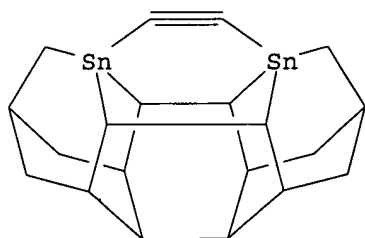
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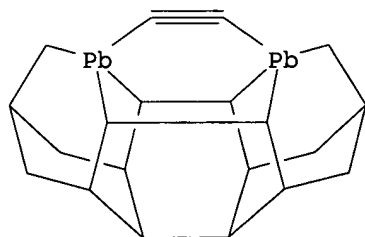
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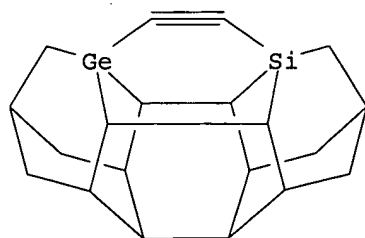
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RN 681029-72-1 HCAPLUS
CN Germasila[6]fulleroid-C22, tetradehydro- (9CI) (CA INDEX NAME)



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DICTIONARY FILE UPDATES: 9 MAR 2005 HIGHEST RN 844817-50-1

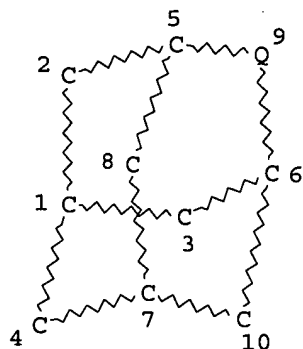
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
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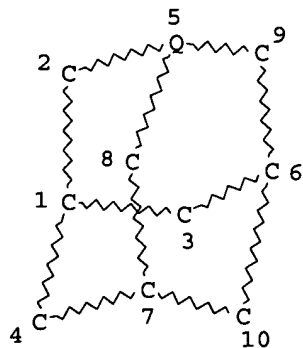
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L47 STR



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NUMBER OF NODES IS 10

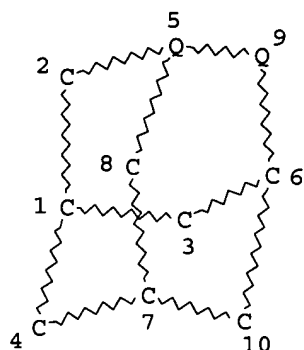
STEREO ATTRIBUTES: NONE
L49 STR



NODE ATTRIBUTES:
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 L51 STR



NODE ATTRIBUTES:
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STEREO ATTRIBUTES: NONE
 L56 SCR 1845
 L57 0 SEA FILE=REGISTRY SSS SAM (L47 OR L49 OR L51) AND L56

3.7% PROCESSED 1000 ITERATIONS 0 ANSWERS
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 524526 TO 544074
 PROJECTED ANSWERS: 0 TO 0

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STRUCTURE FILE UPDATES: 13 MAR 2005 HIGHEST RN 845467-46-1
 DICTIONARY FILE UPDATES: 13 MAR 2005 HIGHEST RN 845467-46-1

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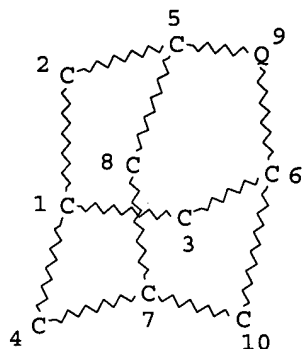
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L1 STR



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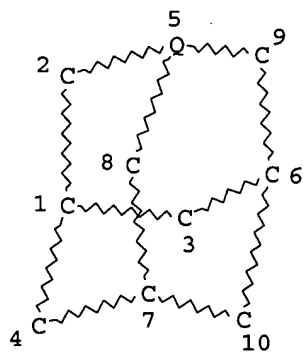
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L2 STR



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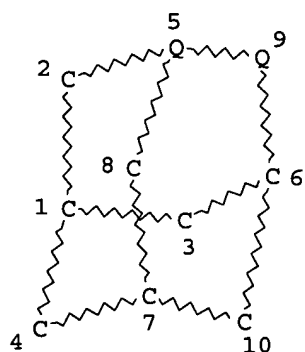
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L3 STR



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GRAPH ATTRIBUTES:
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 NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

L4 SCR 1845

L5 125 SEA FILE=REGISTRY SSS FUL (L1 OR L2 OR L3) AND L4

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125 ANSWERS

SEARCH TIME: 00.00.09

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SET COST OFF

FILE 'REGISTRY' ENTERED AT 06:40:32 ON 14 MAR 2005

ACT SHIAO622A/A

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L1      STR
L2      STR
L3      STR
L4      SCR 1845
L5      125 SEA FILE=REGISTRY SSS FUL (L1 OR L2 OR L3) AND L4

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ACT SHIAO622/A

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L7 (      263)SEA FILE=HCAPLUS ABB=ON  PLU=ON  ?DIAMONDROID?
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L9 (      98)SEA FILE=HCAPLUS ABB=ON  PLU=ON  L7 AND ?AMANTAN?
L10 (     98)SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L8 OR L9)
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L15 (      80)SEA FILE=REGISTRY ABB=ON  PLU=ON  L14 AND ?AMANTAN?/CNS
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L34 16 S L31,L33
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L35 9 S L29 NOT L32
E 2395/RID
L36 19 S E6-E29
E 99573/RID
L37 10 S E3-E13
E 81072/RID
L38 4 S E3-E8
E 7965/RID
L39 54 S E3-E56
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L41 7 S L40 AND (CU OR SI)/ELS
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L44 7 S L29 AND L42
SAV L43 SHIAO622C/A

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L46 0 S L43

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L50 1 S L48,L49
L51 8 S L47,L50

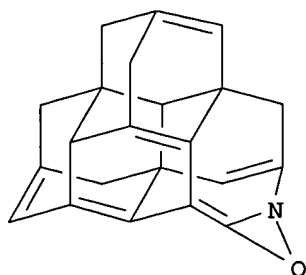
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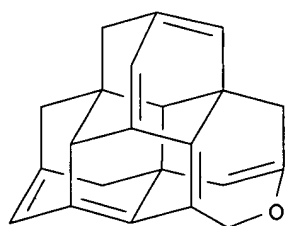
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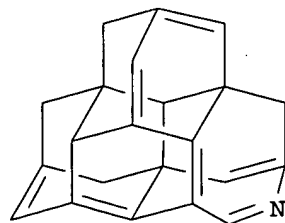
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anthra[9,1-cd]oxazirino[2,3-a]azepine (9CI) (CA INDEX NAME)
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CI RPS
SR CA Index Guide or Ring Systems Handbook



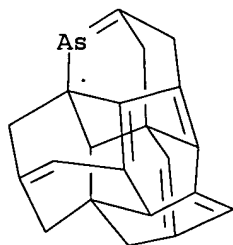
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 MF C22 H16 O
 CI RPS
 SR CA Index Guide or Ring Systems Handbook



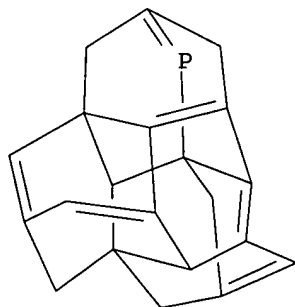
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 RN 656230-40-9 REGISTRY
 CN 5H,8H-3,12:6,14-Dimethano-10,8,4a,12-[1,2]propanediyl[3]ylideneanthra[9,1-cd]azepine (9CI) (CA INDEX NAME)
 MF C22 H15 N
 CI RPS
 SR CA Index Guide or Ring Systems Handbook



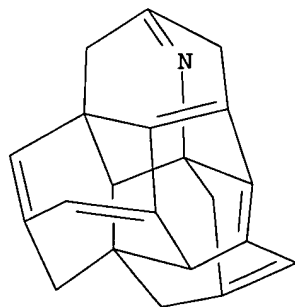
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 RN 656230-39-6 REGISTRY
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 MF C21 H15 As
 CI RPS
 SR CA Index Guide or Ring Systems Handbook



L43 ANSWER 5 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 656230-38-5 REGISTRY
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-naphtho[1,2,3-de]phosphinoline (9CI) (CA INDEX NAME)
MF C21 H15 P
CI RPS
SR CA Index Guide or Ring Systems Handbook



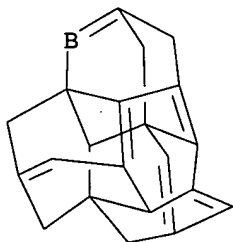
L43 ANSWER 6 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 656230-37-4 REGISTRY
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MF C21 H15 N
CI RPS
SR CA Index Guide or Ring Systems Handbook



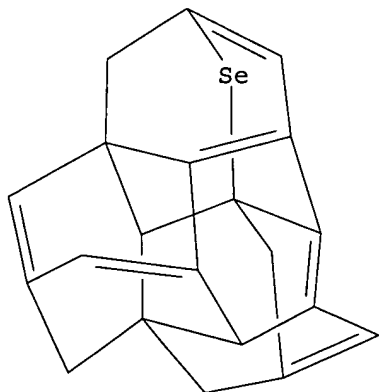
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RN 656230-36-3 REGISTRY

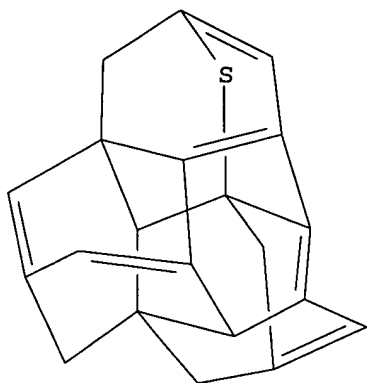
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-anthra[1,9-bc]borin (9CI) (CA INDEX NAME)
MF C21 H15 B
CI RPS
SR CA Index Guide or Ring Systems Handbook



L43 ANSWER 8 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 656230-35-2 REGISTRY
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[1,9-bc]selenin (9CI) (CA INDEX NAME)
MF C21 H14 Se
CI RPS
SR CA Index Guide or Ring Systems Handbook

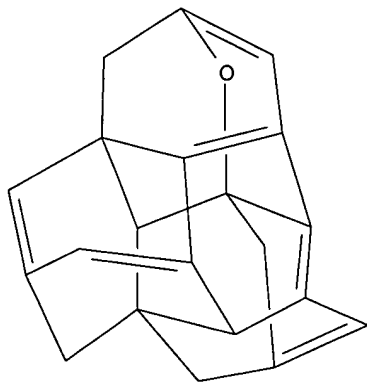


L43 ANSWER 9 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 656230-34-1 REGISTRY
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[1,9-bc]thiopyran (9CI) (CA INDEX NAME)
MF C21 H14 S
CI RPS
SR CA Index Guide or Ring Systems Handbook



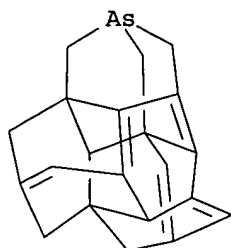
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 MF **C21 H14 O**
 CI RPS
 SR CA Index Guide or Ring Systems Handbook

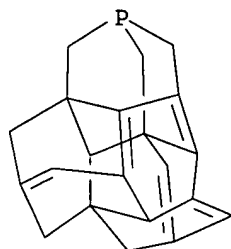


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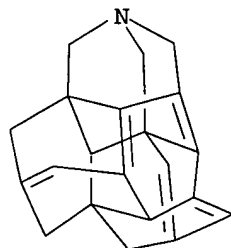
L43 ANSWER 11 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 656230-32-9 REGISTRY
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 MF **C21 H17 As**
 CI RPS
 SR CA Index Guide or Ring Systems Handbook



L43 ANSWER 12 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 656230-31-8 REGISTRY
 CN 3H,4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-dibenz[de,h]isophosphinoline (9CI) (CA INDEX NAME)
 MF C21 H17 P
 CI RPS
 SR CA Index Guide or Ring Systems Handbook



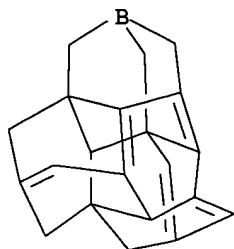
L43 ANSWER 13 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 656230-30-7 REGISTRY
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 MF C21 H17 N
 CI RPS
 SR CA Index Guide or Ring Systems Handbook



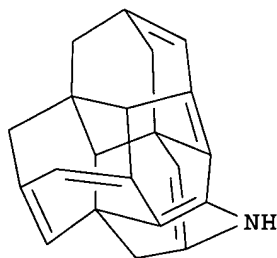
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 MF C21 H17 B

CI RPS
SR CA Index Guide or Ring Systems Handbook

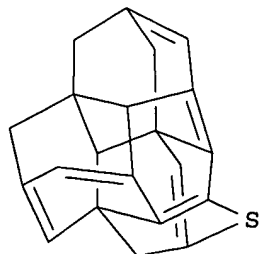


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RN 656230-28-3 REGISTRY
CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylidene-1H-dibenzo[de,h]quinoline (9CI) (CA INDEX NAME)
MF C21 H15 N
CI RPS
SR CA Index Guide or Ring Systems Handbook



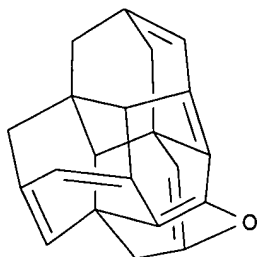
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RN 656230-27-2 REGISTRY
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MF C21 H14 S
CI RPS
SR CA Index Guide or Ring Systems Handbook



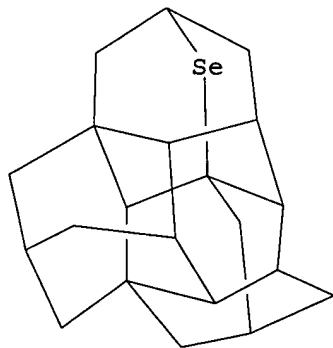
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 MF C21 H14 O
 CI RPS
 SR CA Index Guide or Ring Systems Handbook



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 RN 652999-07-0 REGISTRY
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 MF C21 H26 Se
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL
 DT.CA Caplus document type: Patent
 RL.P Roles from patents: PRP (Properties)



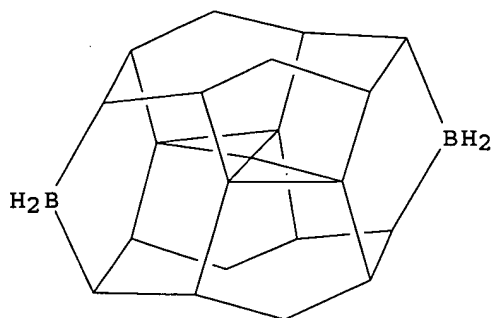
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 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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L43 ANSWER 19 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 475276-89-2 REGISTRY
 CN 1,2:16,20-Diborylene-4,9,14,18-methyno-1,2:6,7:11,12:16,20-tetraseco[5]fullerane-C20-1h, 21,23-dihydro- (9CI) (CA INDEX NAME)

MF C21 H24 B2
SR CA
LC STN Files: CA, CAPLUS
DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: PRP (Properties)



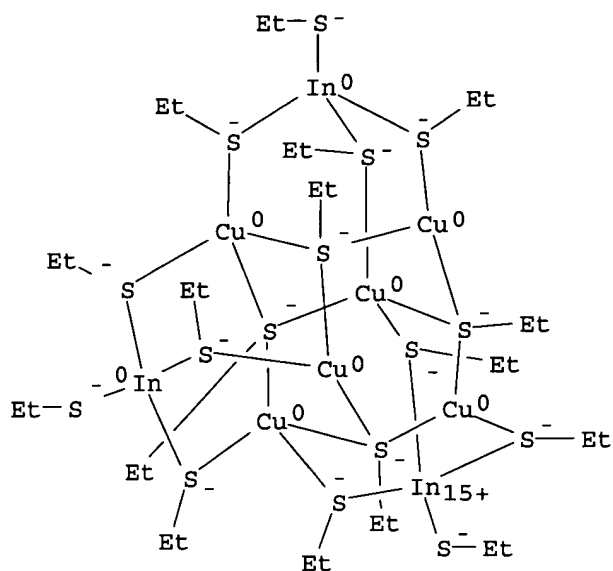
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REFERENCE 1: 137:370137

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RN 142381-39-3 REGISTRY
CN Phosphonium, tetraphenyl-, nonakis[μ-(ethanethiolato)]tetrakis[μ3-(ethanethiolato)]tris[(ethanethiolato)indate]hexacuprate(1-) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Cuprate(1-), nonakis[μ-(ethanethiolato)]tetrakis[μ3-(ethanethiolato)]tris[(ethanethiolato)indate]hexa-, tetraphenylphosphonium (9CI)
MF C32 H80 Cu6 In3 S16 . C24 H20 P
SR CA
LC STN Files: CA, CAPLUS
DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties)

CM 1

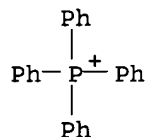
CRN 142381-38-2
CMF C32 H80 Cu6 In3 S16
CCI CCS



CM 2

CRN 18198-39-5

CMF C24 H20 P



1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 117:61532

L43 ANSWER 21 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN

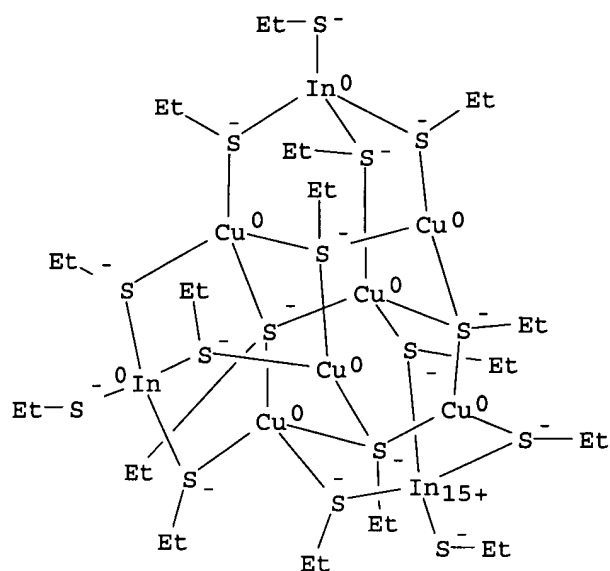
RN 142381-38-2 REGISTRY

CN Cuprate(1-), nonakis[μ-(ethanethiolato)]tetrakis[μ3-(ethanethiolato)]tris[(ethanethiolato)indate]hexa- (9CI) (CA INDEX NAME)

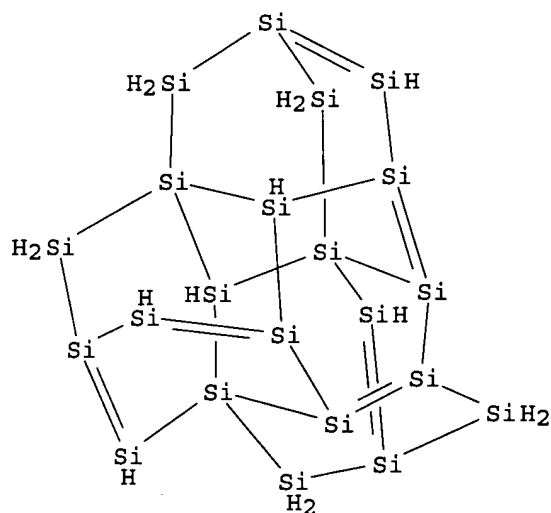
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CI CCS, COM

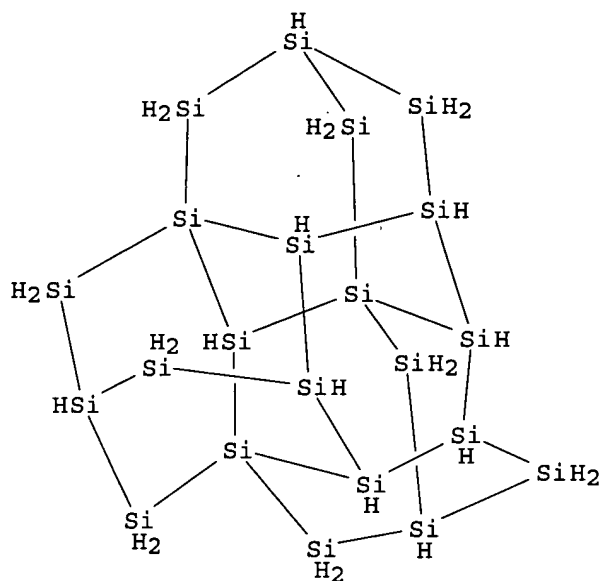
SR CA



L43 ANSWER 22 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 121472-96-6 REGISTRY
 CN 4H,7H-2,11:5,13-Disilano-9,7,3a,11-[1,2]trisilanediy1[3]ylidene-1H-heptadecasilabenz[de]anthracene (9CI) (CA INDEX NAME)
 MF H16 Si22
 CI RPS
 SR CA Index Guide or Ring Systems Handbook



L43 ANSWER 23 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 119052-10-7 REGISTRY
 CN 4H,7H-2,11:5,13-Disilano-9,7,3a,11-[1,2]trisilanediy1[3]ylidene-1H-heptadecasilabenz[de]anthracene, dodecahydro- (9CI) (CA INDEX NAME)
 MF H28 Si22
 SR CA
 LC STN Files: CA, CAPLUS
 DT.CA Caplus document type: Journal
 RL.NP Roles from non-patents: PRP (Properties)



3 REFERENCES IN FILE CA (1907 TO DATE)
 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:173087

REFERENCE 2: 135:10213

REFERENCE 3: 110:86206

L43 ANSWER 24 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN

RN 94396-97-1 REGISTRY

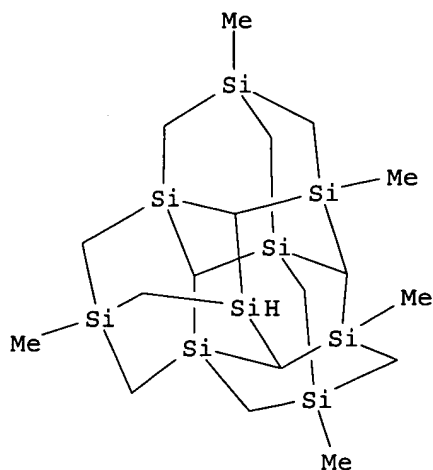
CN 4H,7H-2,11:5,13:9,13-Trimethano-7,3a,11-(silanometheno)-1H-
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 pentamethyl- (9CI) (CA INDEX NAME)

MF C18 H38 Si9

LC STN Files: CA, CAPLUS

DT.CA Caplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation)

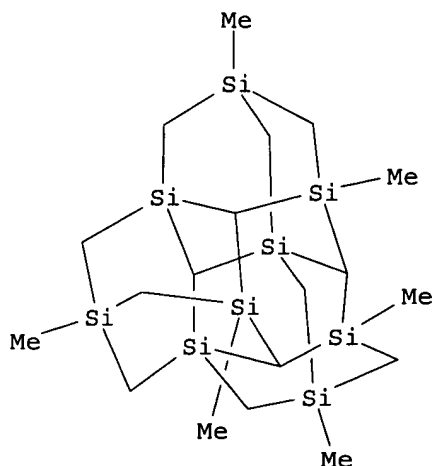


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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 102:78938

L43 ANSWER 25 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN
RN 31714-54-2 REGISTRY
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2,3a,5,6a,7a,9,11,11b-octasilabenz[de]anthracene, dodecahydro-
2,5,6a,7a,9,11b-hexamethyl- (8CI, 9CI) (CA INDEX NAME)
MF C19 H40 Si9
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)
DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)



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REFERENCE 2: 73:56178

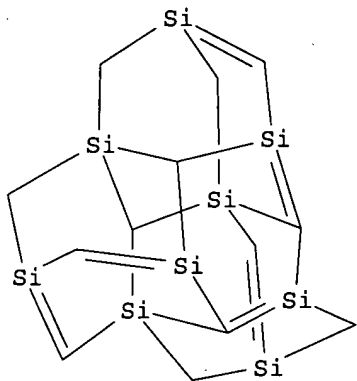
L43 ANSWER 26 OF 26 REGISTRY COPYRIGHT 2005 ACS on STN

RN 29861-92-5 REGISTRY

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2,3a,5,6a,7a,9,11,11b-octasilabenz[de]anthracene (9CI) (CA INDEX NAME)

MF C13 H16 Si9

CI RPS



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CA INDEXING COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 10 Mar 2005 (20050310/PD)

FILE LAST UPDATED: 10 Mar 2005 (20050310/ED)

HIGHEST GRANTED PATENT NUMBER: US6865747

HIGHEST APPLICATION PUBLICATION NUMBER: US2005055750

CA INDEXING IS CURRENT THROUGH 10 Mar 2005 (20050310/UPCA)

ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 10 Mar 2005 (20050310/PD)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2005

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2005

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>>> original, i.e., the earliest published granted patents or <<<
>>> applications. USPAT2 contains full text of the latest US <<<
>>> publications, starting in 2001, for the inventions covered in <<<
>>> USPATFULL. A USPATFULL record contains not only the original <<<
>>> published document but also a list of any subsequent <<<
>>> publications. The publication number, patent kind code, and <<<
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>>> /PK, etc. <<<

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>>> enter this cluster. <<<
>>> <<<
>>> Use USPATALL when searching terms such as patent assignees, <<<
>>> classifications, or claims, that may potentially change from <<<

>>> the earliest to the latest publication.

<<<

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> => d bib abs hitstr 152

L52 ANSWER 1 OF 1 USPATFULL on STN

AN 2004:77366 USPATFULL

TI Heterodiamondoids

IN Liu, Shenggao, Hercules, CA, UNITED STATES

Carlson, Robert M., Petaluma, CA, UNITED STATES

Dahl, Jeremy E., Palo Alto, CA, UNITED STATES

PA CHEVRON USA INC. (U.S. corporation)

PI US 2004059145 A1 20040325

AI US 2003-622130 A1 20030716 (10)

PRAI US 2002-397367P 20020718 (60)

DT Utility

FS APPLICATION

LREP William H. Benz, BURNS, DOANE, SWECKER & MATHIS, L.L.P., P.O. Box 1404,
Alexandria, VA, 22313-1404

CLMN Number of Claims: 37

ECL Exemplary Claim: 1

DRWN 51 Drawing Page(s)

LN.CNT 2469

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention is related to heteroatom containing diamondoids (i.e.,
"heterodiamondoids") which are compounds having a diamondoid nucleus in
which one or more of the diamondoid nucleus carbons has been
substitutionally replaced with a noncarbon atom. These heteroatom
substituents impart desirable properties to the diamondoid. In addition,
the heterodiamondoids are functionalized affording compounds carrying
one or more functional groups covalently pendant therefrom. This
invention is further related to polymerizable functionalized
heterodiamondoids. In a preferred aspect of this invention the
diamondoid nuclei are triamantane and higher diamondoid nuclei. In
another preferred aspect, the heteroatoms are selected to give rise to
diamondoid materials which can serve as n- and p-type materials in
electronic devices can serve as optically active materials.

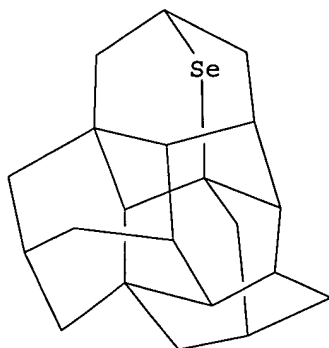
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 652999-07-0

(calcn. of heat of formation; preparation of heterodiamondoids such as aza-,
oxa-, and thiatetramantane from fused adamantanes such as
tetramantanes)

RN 652999-07-0 USPATFULL

CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[1,9-
bc]selenin, dodecahydro- (9CI) (CA INDEX NAME)



=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 07:01:38 ON 14 MAR 2005

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FILE COVERS 1907 - 14 Mar 2005 VOL 142 ISS 12

FILE LAST UPDATED: 13 Mar 2005 (20050313/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d all hitstr tot 151

L51 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:80675 HCAPLUS

DN 140:146009

ED Entered STN: 01 Feb 2004

TI Preparation of heterodiamondoids from fused adamantanes

IN Liu, Shenggao; Carlson, Robert M.

PA Chevron U.S.A. Inc., USA; Dahl, Jeremy E.

SO PCT Int. Appl., 134 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM C07D311-78

ICS C07D313-06; C07D335-04; C07D221-18

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 76

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	WO 2004009577	A1	20040129	WO 2003-US22483	20030717

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 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

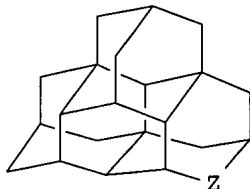
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CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2004009577	ICM	C07D311-78
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US 2004059145	ECLA	C07C023/20; C07C049/423; C07C049/617; C07C061/29; C07D221/22; C07D311/96; C07D313/06; C07D335/04; C07D471/10+221C+221C+9; C07F009/6568C

OS MARPAT 140:146009

GI



I

AB This invention is related to heteroatom containing diamondoids (i.e., 'heterodiamondoids'), e.g. azatetramantane, oxatetramantane, and thiatetramantane (I; X = NH, O, S), which are compds. having a diamondoid nucleus in which one or more of the diamondoid nucleus carbons has been substitutionally replaced with a noncarbon atom. These heteroatom substituents impart desirable properties to the diamondoid. In addition, the heterodiamondoids are functionalized affording compds. carrying one or more functional groups covalently pendant therefrom. This invention is further related to polymerizable functionalized heterodiamondoids. In a preferred aspect of this invention the diamondoid nuclei are triamantane and higher diamondoid nuclei. In another preferred aspect, the heteroatoms are selected to give rise to diamondoid materials which can serve as n- and p-type materials in electronic devices and in optical devices as optically active materials (no data).

ST heterodiamondoid prepn; azatetramantane oxatetramantane thiatetramantane prepn

IT Formation enthalpy

(preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane from fused adamantanes such as tetramantanes)

IT Heterocyclic compounds

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane from fused adamantanes such as tetramantanes)

IT 652998-89-5, [121212121] Decamantane 652998-90-8, [121212121] Oxadecamantane 652998-91-9, [121212121] Thiadecamantane 652998-92-0, [121212121] Selenadecamantane 652998-93-1, [121212121] Boradecamantane 652998-94-2, [121212121] Azadecamantane 652998-95-3, [121212121] Phosphadecamantane 652998-96-4, [121212121] Arsadecamantane

652998-97-5, [1212121212] Undecamantane 652998-98-6, [1212121212]
 Oxaundecamantane 652998-99-7, [1212121212] Thiaundecamantane
 652999-00-3, [1212121212] Selenundecamantane 652999-01-4, [1212121212]
 Boraundecamantane 652999-02-5, [1212121212] Azaundecamantane
 652999-03-6, [1212121212] Phosphaundecamantane 652999-04-7, [1212121212]
 Arsaundecamantane 652999-05-8 652999-06-9 **652999-07-0**
 652999-08-1 652999-09-2 652999-11-6 652999-12-7 652999-35-4
 652999-36-5 652999-38-7 652999-39-8 652999-40-1, [121212121]
 Boradecamantane 652999-41-2, [121212121] Azadecamantane 652999-42-3,
 [121212121] Phosphadecamantane 652999-43-4, [121212121] Arsadecamantane
 652999-44-5, [1212121212] Boraundecamantane 652999-45-6, [1212121212]
 Azaundecamantane 652999-46-7, [1212121212] Phosphaundecamantane
 652999-47-8, [1212121212] Arsaundecamantane

RL: PRP (Properties)

(calcn. of heat of formation; preparation of heterodiamondoids such as aza-,
 oxa-, and thiatetramantane from fused adamantanes such as
 tetramantanes)

IT 917-54-4, Methyllithium 27745-90-0 73635-95-7 73635-96-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane
 from fused adamantanes such as tetramantanes)

IT 546101-72-8P 546102-13-0P 652999-13-8P 652999-14-9P 652999-16-1P
 652999-17-2P 652999-18-3P 652999-19-4P 652999-20-7P 652999-23-0P
 652999-24-1P 652999-25-2P 652999-26-3P 652999-27-4P 652999-29-6P
 652999-30-9P 652999-31-0P 652999-33-2P 652999-34-3P 653570-14-0P
 653570-15-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane
 from fused adamantanes such as tetramantanes)

IT 652999-15-0P 652999-21-8P 652999-22-9P 652999-28-5P 652999-32-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of heterodiamondoids such as aza-, oxa-, and thiatetramantane
 from fused adamantanes such as tetramantanes)

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD

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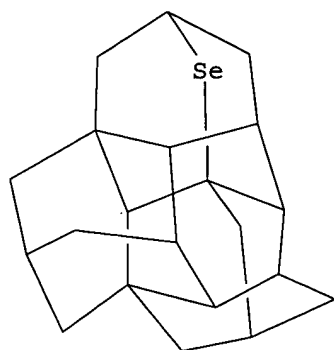
IT **652999-07-0**

RL: PRP (Properties)

(calcn. of heat of formation; preparation of heterodiamondoids such as aza-,
 oxa-, and thiatetramantane from fused adamantanes such as
 tetramantanes)

RN 652999-07-0 HCAPLUS

CN 4H,7H-2,11:5,13-Dimethano-9,7,3a,11-[1,2]propanediyl[3]ylideneanthra[1,9-
 bc]selenin, dodecahydro- (9CI) (CA INDEX NAME)



L51 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2002:685440 HCAPLUS
 DN 137:370137
 ED Entered STN: 11 Sep 2002
 TI The Theoretical Design of Neutral Planar Tetracoordinate Carbon Molecules
 with C(C)4 Substructures
 AU Wang, Zhi-Xiang; Schleyer, Paul von Rague
 CS Computational Chemistry Annex, University of Georgia, Athens, GA,
 30602-2525, USA
 SO Journal of the American Chemical Society (2002), 124(40), 11979-11982
 CODEN: JACSAT; ISSN: 0002-7863
 PB American Chemical Society
 DT Journal
 LA English
 CC 29-4 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 22, 24
 AB Using a new charge-compensation strategy, neutral mols. were designed with
 perfectly planar C(C)4-type tetracoordinate carbon arrangements (ptC)
 employing DFT computations. These designs, based on the planar preference
 of methane dications, replace two remote carbons in spiroalkaplanes by
 borons or two remote hydrogens by BH3 groups; the two formally anionic
 boron units which result compensate the formal double pos. charge on the
 central ptC's. The LUMOs correspond to the "wasted" lone pair HOMOs of
 the alkaplanes. As compared to the latter, π occupancies on the
 central carbon are much smaller (less than 0.7e), and the IPs are much
 larger. The newly predicted compds. utilize all of the electrons more
 effectively. There are no lone pairs, and the ptC-C bond lengths are ca.
 1.50 Å. The Wiberg bond index sums of the ptC's are near 3.2, and the
 boron sums are close to 4.
 ST planar tetracoordinate carbon boron compd DFT; mol electronic structure
 spiroalkaplane boron compd DFT; HOMO planar tetracoordinate carbon boron
 compd DFT
 IT Molecular structure
 (optimized; theor. study of tetracoordinate carbon mols. with C(C)4
 substructures)
 IT Stereochemistry
 (tetrahedral vs. planar; theor. study of tetracoordinate carbon mols.
 with C(C)4 substructures)
 IT Density functional theory
 Electronic structure
 HOMO (molecular orbital)
 Stabilization energy
 (theor. study of tetracoordinate carbon mols. with C(C)4 substructures)
 IT 74-82-8, Methane, properties 157-40-4, Spiropentane 20741-88-2,
 Methane(1+), properties 73353-64-7, Indeno[7,1-cd]indene 101517-28-6,
 Spiro[2.2]pentane, radical ion(1+) 148810-14-4, Methane, radical

ion(2+), properties 179032-57-6, Spiro[2.2]octaplane 251918-68-0
330597-93-8 475276-87-0 475276-88-1 475276-89-2
475276-90-5 475276-91-6 475276-92-7 475276-93-8 475276-94-9
475276-95-0 475276-96-1 475276-97-2 475276-98-3 475467-16-4
475467-22-2

RL: PRP (Properties)

(theor. study of tetracoordinate carbon mols. with C(C)4 substructures)

RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD

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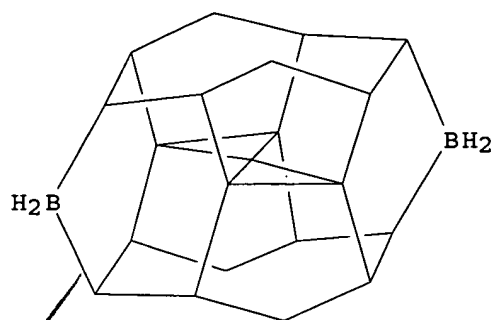
IT 475276-89-2

RL: PRP (Properties)

(theor. study of tetracoordinate carbon mols. with C(C)4 substructures)

RN 475276-89-2 HCAPLUS

CN 1,2:16,20-Diborylene-4,9,14,18-methyno-1,2:6,7:11,12:16,20-
tetraseco[5]fullerane-C20-Ih, 21,23-dihydro- (9CI) (CA INDEX NAME)



L51 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2001:892659 HCAPLUS
 DN 136:173087
 ED Entered STN: 12 Dec 2001
 TI Size, Order, and Dimensional Relations for Silicon Cluster
 Polarizabilities
 AU Jansik, B.; Schimmelpfennig, B.; Norman, P.; Mochizuki, Y.; Luo, Y.;
 Aagren, H.
 CS Theoretical Chemistry, Royal Institute of Technology, Stockholm, S-106 91,
 Swed.
 SO Journal of Physical Chemistry A (2002), 106(2), 395-399
 CODEN: JPCAFH; ISSN: 1089-5639
 PB American Chemical Society
 DT Journal
 LA English
 CC 65-5 (General Physical Chemistry)
 AB Response theory calcns. in the RPA are applied to linear polarizabilities
 and second hyperpolarizabilities of 1-, 2-, and 3-dimensional
 hydrogen-terminated silicon clusters. Successive enlargement of the
 clusters to embody on the order of 50 silicon atoms plus bond-saturating
 hydrogen atoms allows for extrapolation to bulk values of individual
 silicon atom contributions in the 1D and 3D cases. Modern effective core
 potentials are shown to provide excellent approxns. to the all-electron
 values in all cases; errors for both polarizabilities and
 hyperpolarizabilities are on the order of 1%. The findings indicate
 considerable time savings in predictions of the elec. polarizability
 properties of elements beyond the first row atoms.
 ST silicon cluster hydrogen termination polarizability hyperpolarizability
 response theory RPA; effective core potential silicon cluster hydrogen
 termination polarizability hyperpolarizability
 IT Basis sets
 (effective core potential; in study of polarizabilities and
 hyperpolarizabilities of hydrogen-terminated silicon clusters with
 size, order, and dimensional relations studied by response theory in
 RPA)
 IT Electron correlation
 (in study of polarizabilities and hyperpolarizabilities of
 hydrogen-terminated silicon clusters with size, order, and dimensional
 relations studied by response theory in RPA)
 IT Cluster structure
 Hyperpolarizability
 Polarizability
 (of hydrogen-terminated silicon clusters with size, order, and
 dimensional relations studied by response theory in RPA)
 IT Clusters
 Size effect
 (polarizabilities and hyperpolarizabilities of hydrogen-terminated
 silicon clusters with size, order, and dimensional relations studied by

response theory in RPA)

IT Silanes
 RL: PRP (Properties)
 (polarizabilities and hyperpolarizabilities of hydrogen-terminated silicon clusters with size, order, and dimensional relations studied by response theory in RPA)

IT 291-59-8, Cyclohexasilane 1590-87-0, Silicon hydride (Si₂H₆)
 7783-26-8, Silicon hydride (Si₃H₈) 7783-29-1, Silicon hydride (Si₄H₁₀)
 14693-61-9, Hexasilane 39517-09-4, Octasilane 41518-75-6, Decasilane
 72244-91-8, Tetradecasilane 94570-81-7, Triacontasilane 99759-72-5,
 Hexasilabenzene 119052-10-7 128171-51-7, Eicosasilane
 133754-37-7, Hexadecasilane 153549-12-3, Pentadecasilane 155101-73-8,
 Tricyclo[3.3.1.1^{3,7}]decasilane 209683-92-1, Dodecasilane 226714-57-4
 334939-73-0, Silicon hydride (Si₃₅H₃₆) 340809-92-9 397250-81-6,
 Dopentacontasilane 397250-82-7, Hexadecasilapyrene 397250-83-8,
 Tetracosasilacoronene 397250-84-9 397250-85-0, Silicon hydride
 (Si₅₄H₅₆)
 RL: PRP (Properties)
 (polarizabilities and hyperpolarizabilities of hydrogen-terminated silicon clusters with size, order, and dimensional relations studied by response theory in RPA)

RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD

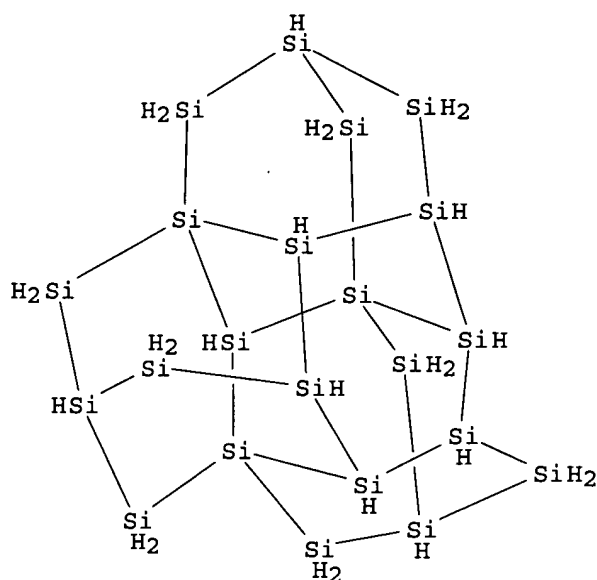
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IT 119052-10-7
 RL: PRP (Properties)
 (polarizabilities and hyperpolarizabilities of hydrogen-terminated silicon clusters with size, order, and dimensional relations studied by response theory in RPA)

RN 119052-10-7 HCAPLUS

CN 4H,7H-2,11:5,13-Disilano-9,7,3a,11-[1,2]trisilanediy1[3]ylidene-1H-heptadecasilabenz[de]anthracene, dodecahydro- (9CI) (CA INDEX NAME)



✓ L51 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2001:207328 HCAPLUS
 DN 135:10213
 ED Entered STN: 22 Mar 2001
 TI Polarizability of silicon clusters
 AU Mochizuki, Y.; Agren, H.
 CS CCSE, Japan Atomic Energy Research Institute, Meguro-ku, Tokyo, 153-0061, Japan
 SO Chemical Physics Letters (2001), 336(5,6), 451-456
 CODEN: CHPLBC; ISSN: 0009-2614
 PB Elsevier Science B.V.
 DT Journal
 LA English
 CC 65-5 (General Physical Chemistry)
 Section cross-reference(s): 76
 AB The polarizability of hydrogen-terminated silicon clusters derived from the silicon diamond-lattice structure was evaluated by linear response calcns. The dependences on cluster size and basis set were systematically investigated. A convergence in calculated polarizability per silicon atom toward the bulk value was found. Frequency-dependent polarizabilities were also addressed.
 ST polarizability silicon cluster
 IT Cluster structure
 Polarizability
 (polarizability of silicon clusters)
 IT 291-59-8, Cyclohexasilane 7440-21-3, Silicon, properties
 119052-10-7 147207-30-5, Silicon hydride (Si35H36)
 212783-55-6, Silicon hydride (Si5H) 226714-57-4 312613-06-2, Silicon hydride (Si10H16) 340809-92-9
 RL: PRP (Properties)
 (polarizability of silicon clusters)
 RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
 RE
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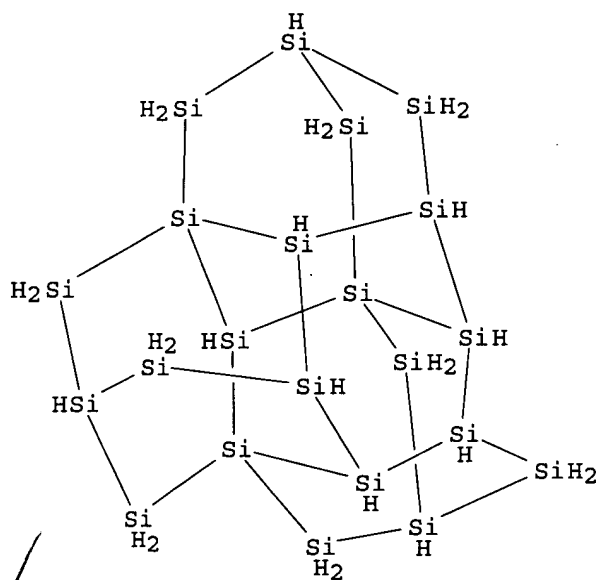
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IT 119052-10-7

RL: PRP (Properties)
(polarizability of silicon clusters)

RN 119052-10-7 HCAPLUS

CN 4H,7H-2,11:5,13-Disilano-9,7,3a,11-[1,2]trisilanediy1[3]ylidene-1H-heptadecasilabenz[de]anthracene, dodecahydro- (9CI) (CA INDEX NAME)



L51 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1992:461532 HCAPLUS

DN 117:61532

ED Entered STN: 08 Aug 1992

TI Synthesis and structure of the first indium-copper cluster,
[Cu₆In₃(SEt)₁₆]- and its possible relevance to CuInS₂

AU Hirpo, Wakgari; Dhingra, Sandeep; Kanatzidis, Mercouri G.

CS Cent. Fundam. Mater. Res., Michigan State Univ., East Lansing, MI, 48824,
USASO Journal of the Chemical Society, Chemical Communications (1992), (7),
557-9

CODEN: JCCCAT; ISSN: 0022-4936

DT Journal

LA English

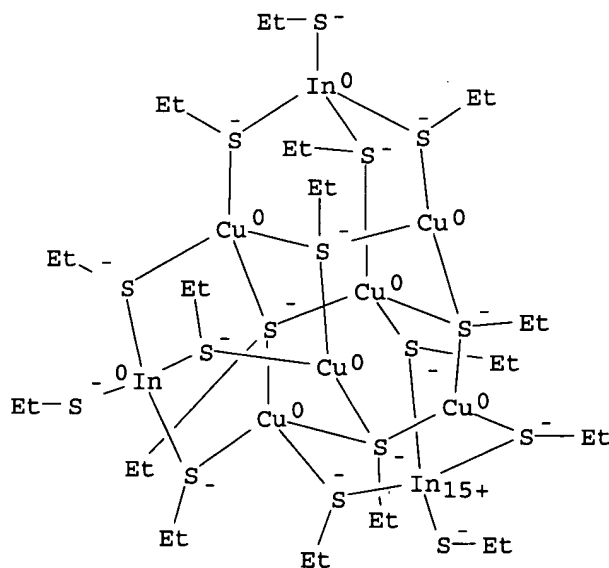
CC 78-7 (Inorganic Chemicals and Reactions)
 Section cross-reference(s): 75
 AB (Ph₄P)[Cu₆In₃(SEt)₁₆] was prepared by the reaction of [Cu(MeCN)₄]PF₆ with
 (Ph₄P)[In(SEt)₄] and its crystal structure shows an adamantoid framework.
 ST crystal structure copper indium ethanethiolato cluster; thiolato copper
 indium nonanuclear cluster
 IT Crystal structure
 Molecular structure
 (of copper indium ethanethiolato nonanuclear cluster)
 IT Cluster compounds, coordinative
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (copper-indium-sulfur, ethanethiolato, preparation and crystal structure of)
 IT **142381-39-3P**
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and crystal structure of)
 IT 142029-65-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with copper acetonitrile complex)
 IT 64443-05-6, Tetrakis(acetonitrile)copper(1+) hexafluorophosphate(1-)
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with indate ethanethiolato complex)
 IT **142381-39-3P**
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and crystal structure of)
 RN 142381-39-3 HCAPLUS
 CN Phosphonium, tetraphenyl-, nonakis[μ-(ethanethiolato)]tetrakis[μ₃-
 (ethanethiolato)]tris[(ethanethiolato)indate]hexacuprate(1-) (9CI) (CA
 INDEX NAME)

CM 1

CRN 142381-38-2

CMF C32 H80 Cu6 In3 S16

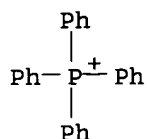
CCI CCS



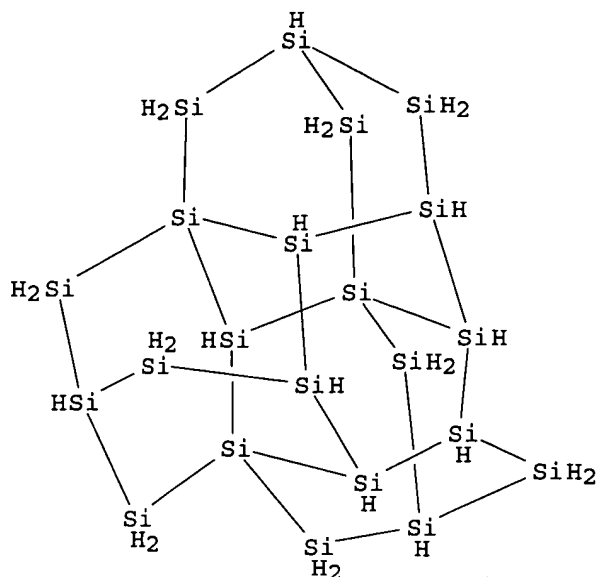
CM 2

CRN 18198-39-5

CMF C24 H20 P



L51 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1989:86206 HCAPLUS
 DN 110:86206
 ED Entered STN: 04 Mar 1989
 TI Hyperfine interactions in cluster models of the Pb defect center
 AU Cook, Michael; White, C. T.
 CS Nav. Res. Lab., Washington, DC, 20375-5000, USA
 SO Physical Review B: Condensed Matter and Materials Physics (1988), 38(14),
 9674-85
 CODEN: PRBMDO; ISSN: 0163-1829
 DT Journal
 LA English
 CC 76-1 (Electric Phenomena)
 AB Hyperfine interactions in the Pb center (denoted schematically as
 Si3.tplbond.Si.), an electron trap, at the Si(111)/SiO2 interface have
 been studied with use of spin-polarized self-consistent
 multiple-scattering X α calcns. on Si22H21/Si6O18H6 and Si22H27
 cluster models. The theor. hyperfine tensor agrees very well with experiment
 when the trivalent atom Si' is relaxed by a value typical of geometries
 found for the neutral paramagnetic charge state in semiempirical and ab
 initio cluster calcns. Spin-polarization effects are very important for a
 detailed description of the Pb defect, particularly with respect to the
 hyperfine couplings at nuclei close to the defect atom. The largest such
 superhyperfine interaction is produced not by the nearest-neighbor atoms
 as has commonly been assumed, but by 3 second-nearest neighbors located
 below Si' in the bulk c-Si. The isotropic and anisotropic superhyperfine
 components and the direction of the principle axes predicted by the
 present calcns. have been confirmed by recent ESR expts.
 ST interface silicon silica hyperfine interaction center
 IT Trapping and Traps
 (at silicon interface with silicon, cluster model of center for)
 IT Interface
 (silica-silicon, Pb center hyperfine interaction at, spin-polarized
 self-consistent multiple-scattering X α calcn. on)
 IT 7440-21-3, Silicon, properties
 RL: PRP (Properties)
 (defect center hyperfine interaction at interface of silica with)
 IT 7631-86-9, Silica, properties
 RL: PRP (Properties)
 (defect center hyperfine interaction at interface of silicon with)
 IT 119052-09-4 **119052-10-7**
 RL: PRP (Properties)
 (interface defect center hyperfine interaction at silicon-silica
 interface from cluster model of)
 IT **119052-10-7**
 RL: PRP (Properties)
 (interface defect center hyperfine interaction at silicon-silica
 interface from cluster model of)
 RN 119052-10-7 HCAPLUS
 CN 4H,7H-2,11:5,13-Disilano-9,7,3a,11-[1,2]trisilanediy1[3]ylidene-1H-
 heptadecasilabenz[de]anthracene, dodecahydro- (9CI) (CA INDEX NAME)



L51 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1985:78938 HCAPLUS
 DN 102:78938
 ED Entered STN: 09 Mar 1985
 TI Formation of organosilicon compounds. 100. Isolation of higher molecular weight carbosilanes from the pyrolysis of tetramethylsilane
 AU Fritz, G.; Woerns, K. P.
 CS Inst. Anorg. Chem., Univ. Karlsruhe, Karlsruhe, D-7500, Fed. Rep. Ger.
 SO Zeitschrift fuer Anorganische und Allgemeine Chemie (1984), 512, 103-25
 CODEN: ZAACAB; ISSN: 0044-2313
 DT Journal
 LA German
 CC 29-6 (Organometallic and Organometalloidal Compounds)
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A systematic investigation of the carbosilanes containing 6 to 9 Si atoms per mol. formed by pyrolysis of SiMe₄ was achieved by means of column chromatog. sepns. combined with HPLC. Eleven pure compds. and mixts. of I (R = Me, R₁ = CH₂SiMe₂CH₂SiMe₃; R = R₁ = Me₃SiCH₂) as well as of II and III were isolated. The predominant structure is that of the carborundanes using only Me and H as Si substituents. Only in compds. IV and V are some of the Si-C 6-membered rings in the chair form. In compds. such as VI another possibility of connecting 1,3,5,7-tetrasiladamantane frameworks to higher mol. carbosilanes is realized.
 ST silane tetramethyl pyrolysis; pyrolysis methylsilane; polycyclic carbosilane; silane siladamantane poly
 IT Chromatography, column and liquid
 (high-performance, isolation of high mol. weight carbosilanes from the pyrolysis of tetramethylsilane by)
 IT 26393-20-4P 31714-54-2P 94396-94-8P 94396-95-9P
 94396-96-0P 94396-97-1P 94396-98-2P 94396-99-3P
 94397-00-9P
 RL: PREP (Preparation)
 (isolation of, from pyrolysis of tetramethylsilane)

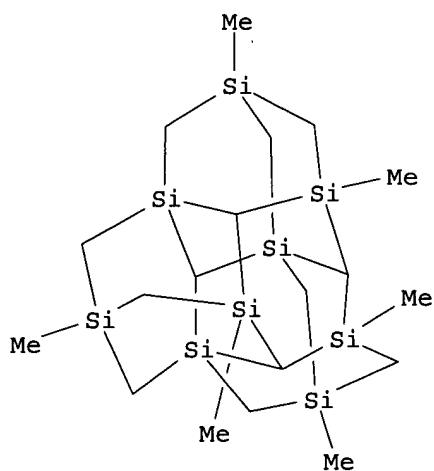
IT 50938-70-0P 65000-98-8P 86932-03-8P 94396-90-4P 94396-91-5P
 94396-92-6P 94396-93-7P 94411-13-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, by pyrolysis of tetramethylsilane)

IT 75-76-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (pyrolysis of, isolation of higher mol. weight carbosilanes from)

IT 31714-54-2P 94396-97-1P
 RL: PREP (Preparation)
 (isolation of, from pyrolysis of tetramethylsilane)

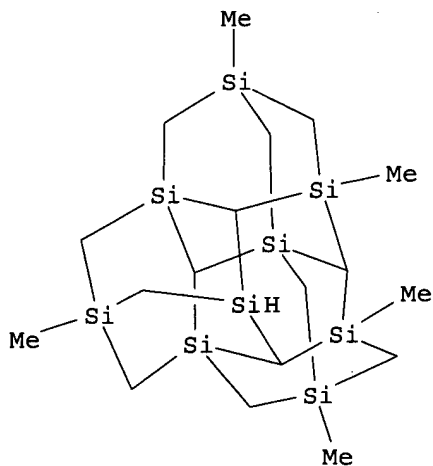
RN 31714-54-2 HCAPLUS

CN 4H,7H-2,11:5,13:9,13-Trimethano-7,3a,11-(silanometheno)-1H-
 2,3a,5,6a,7a,9,11,11b-octasilabenz[de]anthracene, dodecahydro-
 2,5,6a,7a,9,11b-hexamethyl- (8CI, 9CI) (CA INDEX NAME)

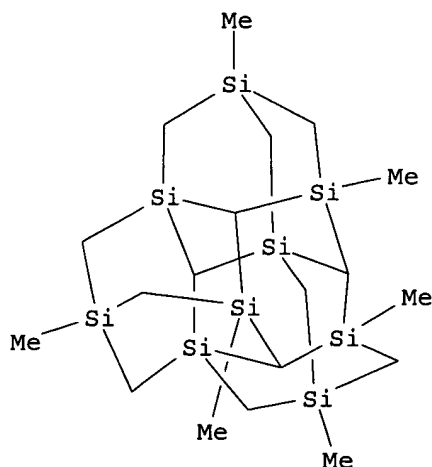


RN 94396-97-1 HCAPLUS

CN 4H,7H-2,11:5,13:9,13-Trimethano-7,3a,11-(silanometheno)-1H-
 2,3a,5,6a,7a,9,11,11b-octasilabenz[de]anthracene, dodecahydro-2,5,6a,7a,9-
 pentamethyl- (9CI) (CA INDEX NAME)



DN 73:56178
 ED Entered STN: 12 May 1984
 TI Silicon-carbon compounds with a carborundum structure ("carborundanes")
 AU Fritz, Gerhard; Diem, Fritz; Koehler, Helmut; Kummer, Dieter; Scheer, Heinz
 CS Inst. Anorg. Chem., Univ. Karlsruhe, Karlsruhe, Fed. Rep. Ger.
 SO Angewandte Chemie, International Edition in English (1970), 9(6), 464-5
 CODEN: ACIEAY; ISSN: 0570-0833
 DT Journal
 LA English
 CC 29 (Organometallic and Organometalloidal Compounds)
 GI For diagram(s), see printed CA Issue.
 AB 1,3,5,7-Tetramethyl-1,3,5,7-tetrasilatricyclo [3.3.1.1^{3,7}]decane (I) and small amts. 1,3,7,9,11,13-hexamethyl-1,3,5,7,9,11,13-heptasilahexacyclo [7.5.1.1^{3,13}.1^{7,11}.0^{5,12}.0^{5,15}]heptadecane (II), 3,7,11,13,15,17-hexamethyl-1,3,5,7,9,11,13,15,17-enneasilaenneacyclo [9.1.7.1^{11,5}.1^{3,17}.1^{7,15}.0^{5,16}.0^{9,14}.0^{9,20}.1^{3,18}] docosane (III), and 3,7,11,17-tetramethyl-1,3,5,7,9,11,13,15,17,19-decasilaundecacyclo [9.9.1.1^{11,5}.1^{3,19}.1^{5,19}.1^{7,15}.1^{13,17}.0^{9,14}.0^{9,22}.1^{3,20}.1^{5,24}]hexacosane (IV) are obtained when SiMe₄ is pyrolyzed (700°). NMR data for II-IV are given.
 ST carborundanes silicon carbon compds; silicon carbon compds carborundanes; carbon silicon compds carborundanes; silaadamantanes; adamantanes sila; methyl silanes pyrolysis; silanes methyl pyrolysis; pyrolysis methyl silanes
 IT 26393-20-4P 31714-54-2P 32069-85-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 IT 31714-54-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 31714-54-2 HCAPLUS
 CN 4H,7H-2,11:5,13:9,13-Trimethano-7,3a,11-(silanometheno)-1H-2,3a,5,6a,7a,9,11,11b-octasilabenz[de]anthracene, dodecahydro-2,5,6a,7a,9,11b-hexamethyl- (8CI, 9CI) (CA INDEX NAME)



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